High Performance Computing (HPC) Introduction

Ontario Summer School on
High Performance Computing

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SciNet HPC Consortium

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Outline

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Acknowledgments

Contributing Material

- Intro to HPC - S. Northrup, M. Ponce, SciNet
- SciNet Parallel Scientific Computing Course - L. J. Dursi & R. V. Zon, SciNet
- Parallel Computing Models - D. McCaughan, SHARCNET
- High Performance Computing - D. McCaughan, SHARCNET
- HPC Architecture Overview - H. Merez, SHARCNET
- Intro to HPC - T. Whitehead, SHARCNET

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Outline

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Scientific High Performance Computing

What is it?

HPC is essentially leveraging larger and/or multiple computers to solve computations in parallel.

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What does it involve?

- hardware - pipelining, instruction sets, multi-processors, inter-connects
- algorithms - concurrency, efficiency, communications
- software - parallel approaches, compilers, optimization, libraries

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When do I need HPC?

- My problem takes too long $\rightarrow$ more/faster computation
- My problem is too big $\rightarrow$ more memory
- My data is too big $\rightarrow$ more storage

Scientific High Performance Computing

Why is it necessary?

- Modern experiments and observations yield vastly more data to be processed than in the past.
- As more computing resources become available, the bar for cutting edge simulations is raised.
- Science that could not have been done before becomes tractable.

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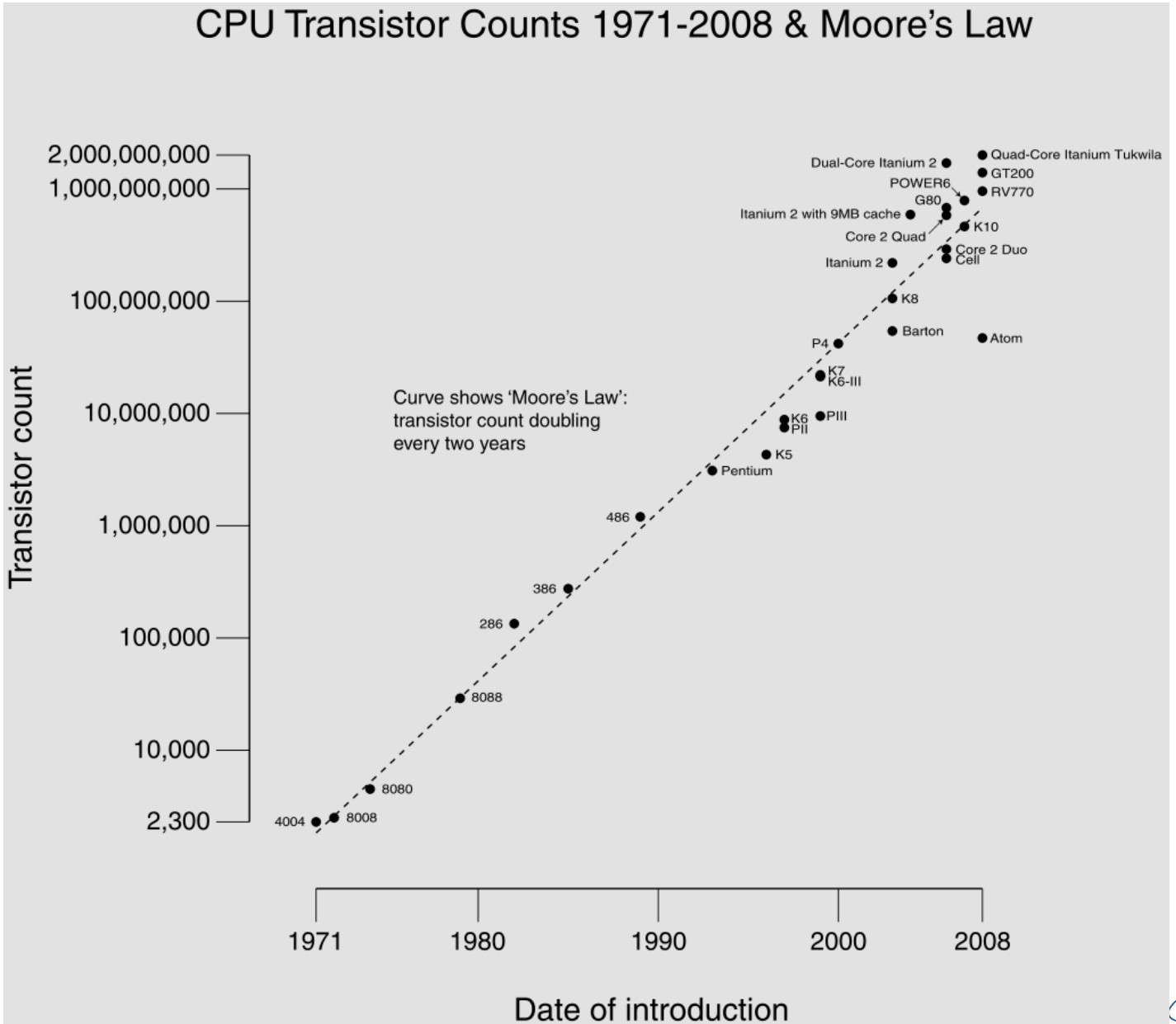
However

- Advances in clock speeds, bigger and faster memory and storage have been lagging as compared to e.g. 10 years ago. *Can no longer "just wait a year" and get a better computer.*
- So modern HPC means more hardware, not faster hardware.
- Thus parallel programming/computing is required.

Wait, what about Moore's Law?



(source: Transistor Count and Moore's Law - 2008.svg, by Wgsimon, wikipedia)

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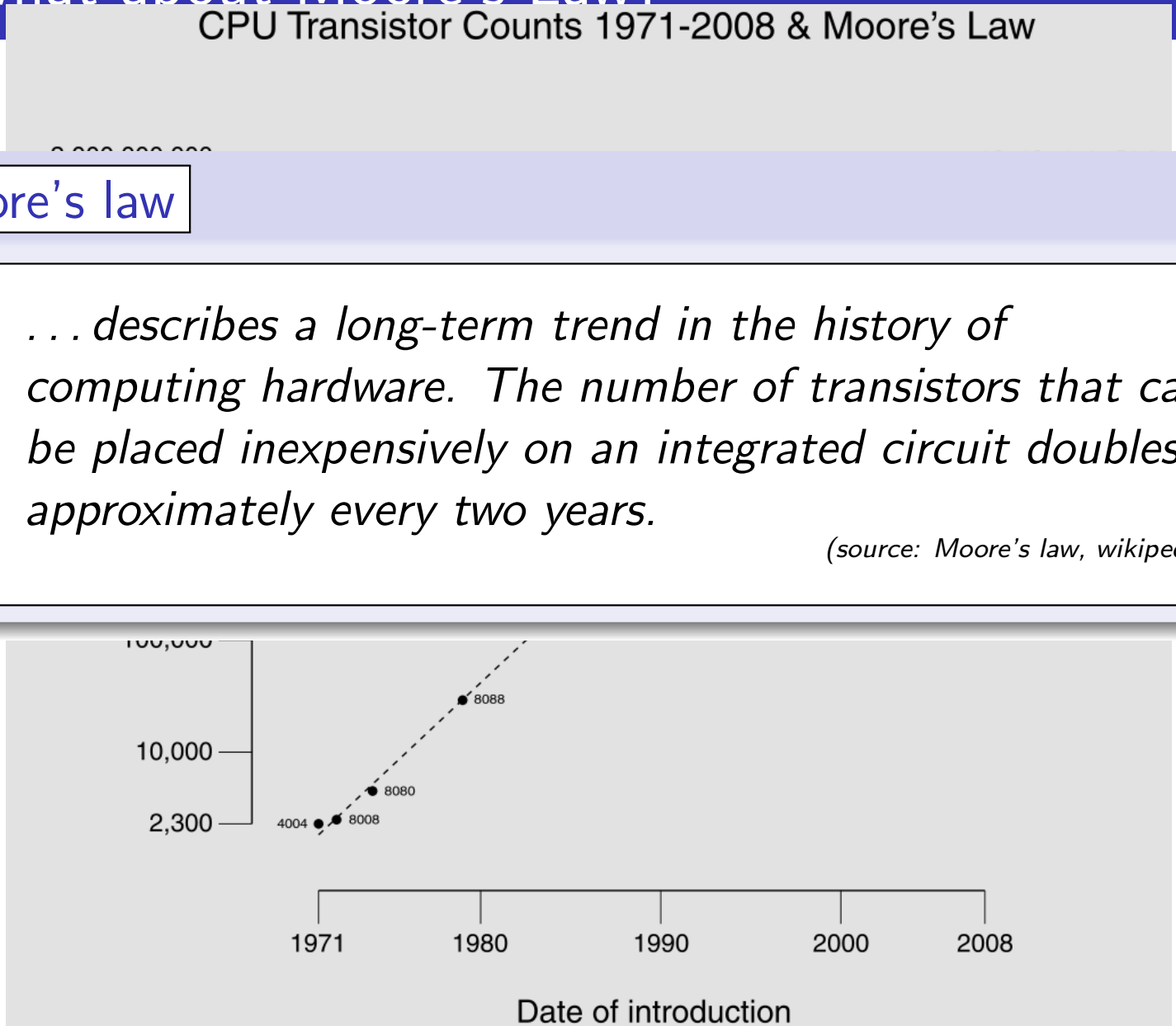
Wait, what about Moore's Law?



Moore's law

. . . describes a long-term trend in the history of computing hardware. The number of transistors that can be placed inexpensively on an integrated circuit doubles approximately every two years.

(source: Moore's law, wikipedia)

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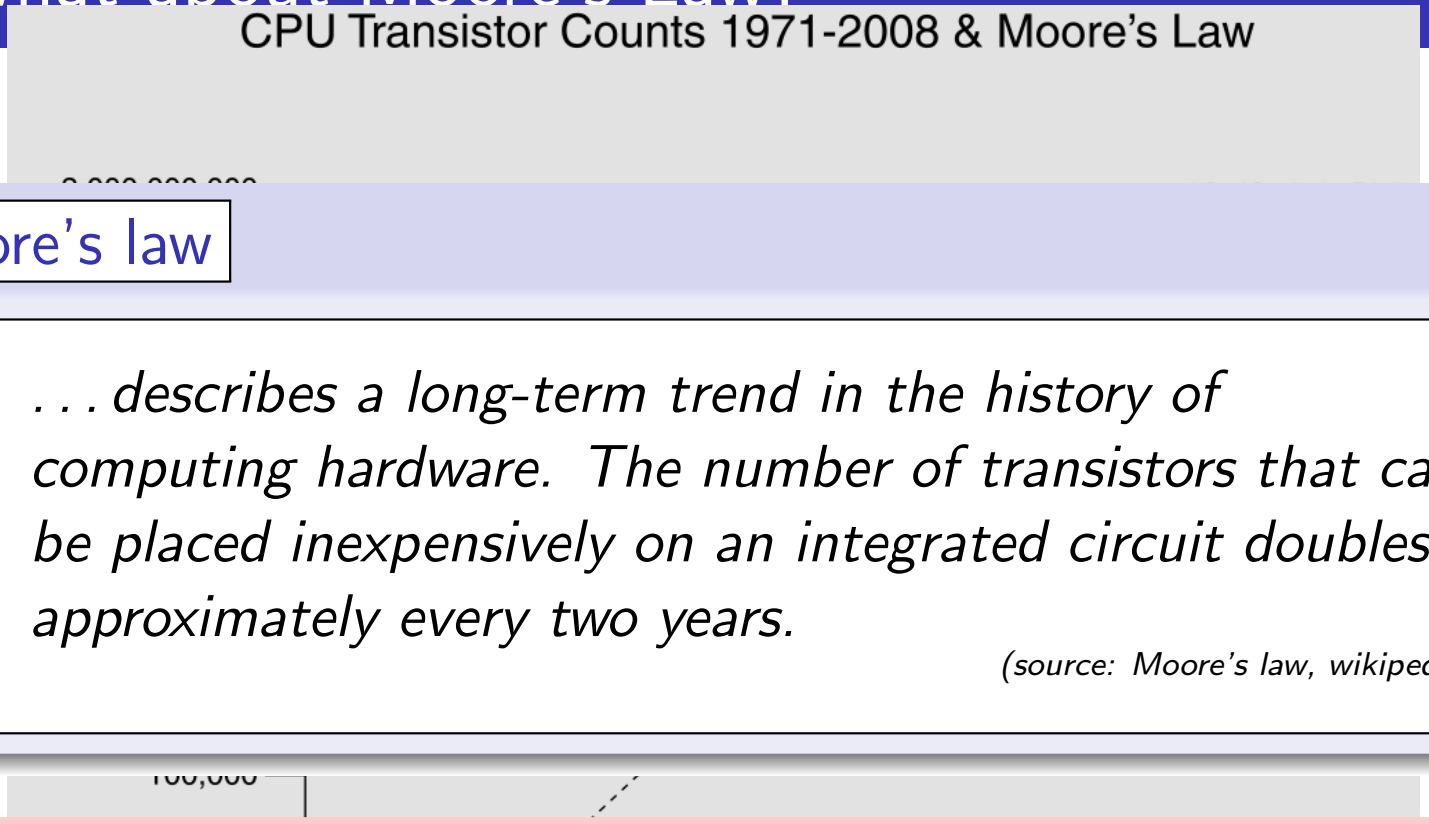

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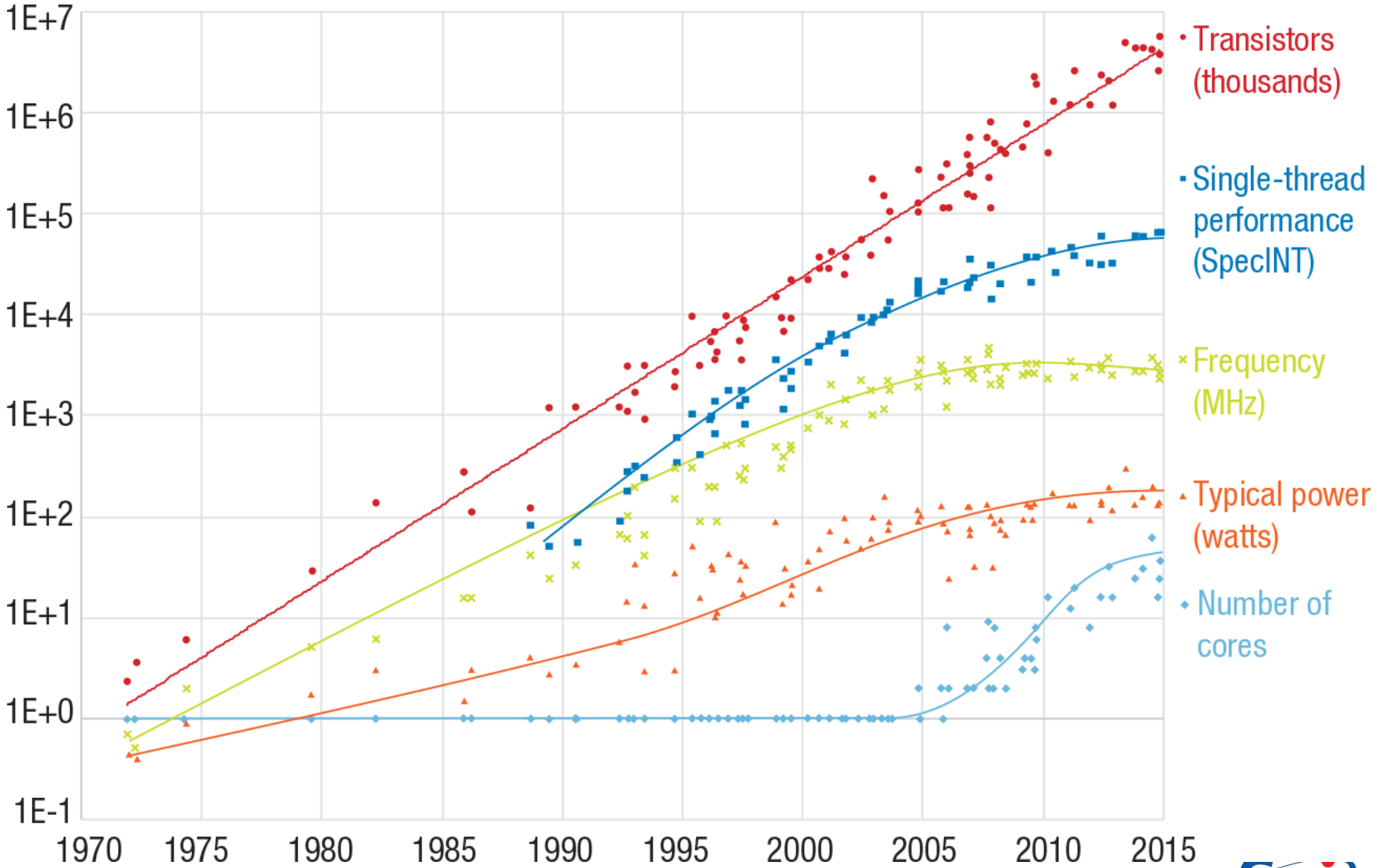
(source: Moore's law, wikipedia)

But. . .

- *Moore's Law didn't promise us clock speed.*
- *More transistors but getting hard to push clockspeed up. Power density is limiting factor.*
- *So more cores at fixed clock speed.*

Easy performance gains coming to an end



(source: Bresniker, Singhal, & Williams, Computer vol. 48 no. 12, p44-53, 2015)

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Analogy

HR Dilemma

- Problem: job needs to get done faster

Analogy

HR Dilemma

- Problem: job needs to get done faster
  - can't hire substantially faster people
  - can hire more people

Analogy

HR Dilemma

- Problem: job needs to get done faster
  - can't hire substantially faster people
  - can hire more people
- Solution:
  - split work up between people (divide and conquer)
  - requires rethinking the work flow process
  - requires administration overhead
  - eventually administration larger than actual work

Outline

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Parallel Computing

Thinking Parallel

The general idea is if one processor is good, many processors will be better

- Parallel programming is not generally trivial
- Tools for automated parallelism are either highly specialized or absent
- serial algorithms/mathematics don't always work well in parallel without modification

Parallel Computing

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Parallel Programming

- it's Necessary (serial performance has peaked)
- it's Everywhere (cellphones, tablets, laptops, etc)
- it's still increasing (Sequoia 1.5 M cores, Tianhe-2 3.12M cores)

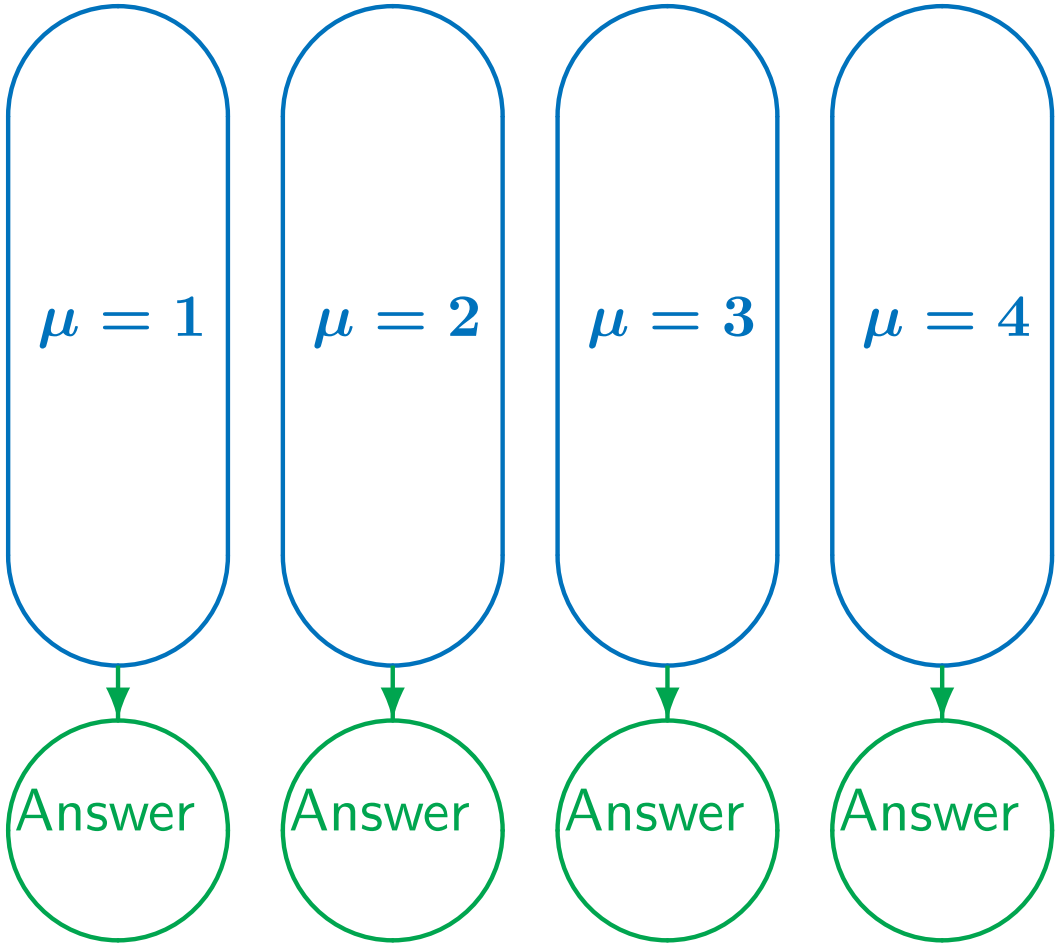
Concurrency

- Must have something to do for all these cores.
- Find parts of the program that can done independently, and therefore concurrently.
- There must be many such parts.
- Their order of execution should not matter either.
- Data dependencies limit concurrency.

(source: http://flickr.com/photos/splorp)

Parameter study: best case scenario

- Aim is to get results from a model as a parameter varies.
- Can run the serial program on each processor at the same time.
- Get "more" done.



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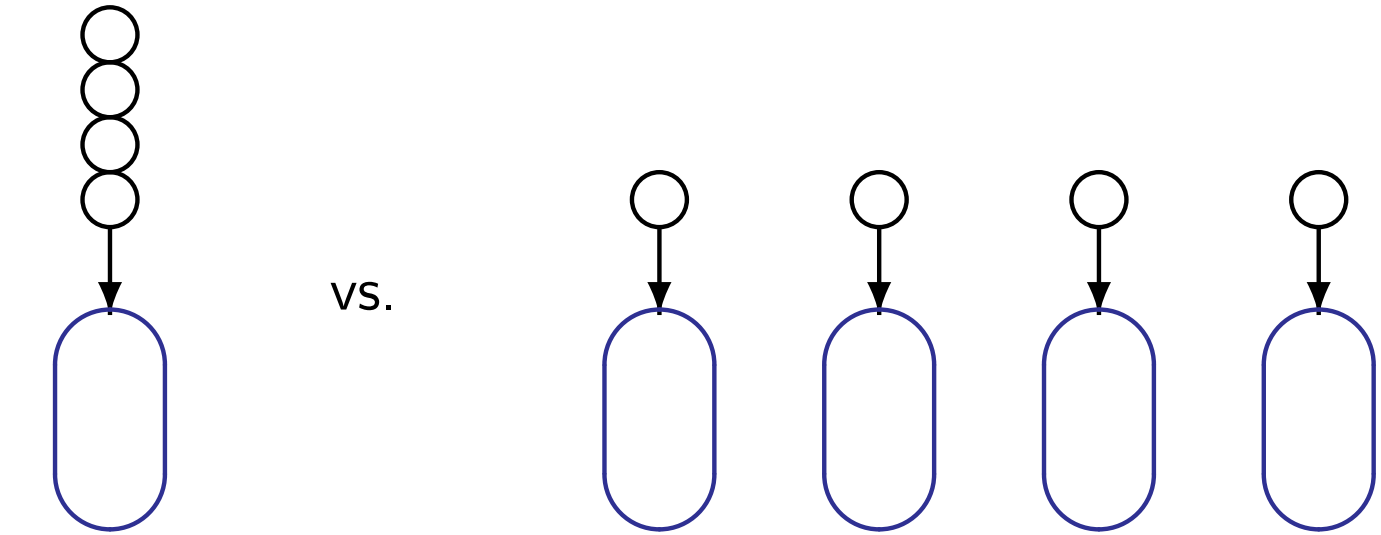
Throughput

- How many tasks can you do per unit time?

$$\text{throughput} = \boldsymbol{H} = \frac{\boldsymbol{N}}{\boldsymbol{T}}$$

- Maximizing $\boldsymbol{H}$ means that you can do as much as possible.
- Independent tasks: using $\boldsymbol{P}$ processors increases $\boldsymbol{H}$ by a factor $\boldsymbol{P}$



$\boldsymbol{T = NT_1}$
$\boldsymbol{H = 1/T_1}$

$\boldsymbol{T = NT_1/P}$
$\boldsymbol{H = P/T_1}$

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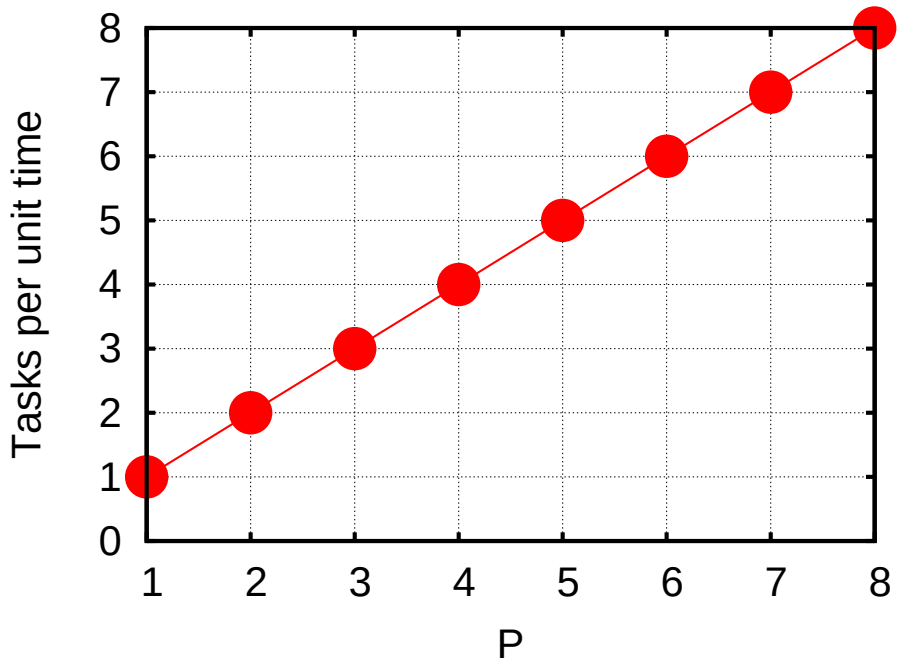
Scaling — Throughput

- How a problem's throughput scales as processor number increases ("strong scaling").
- In this case, linear scaling:

$$H \propto P$$

- This is Perfect scaling.

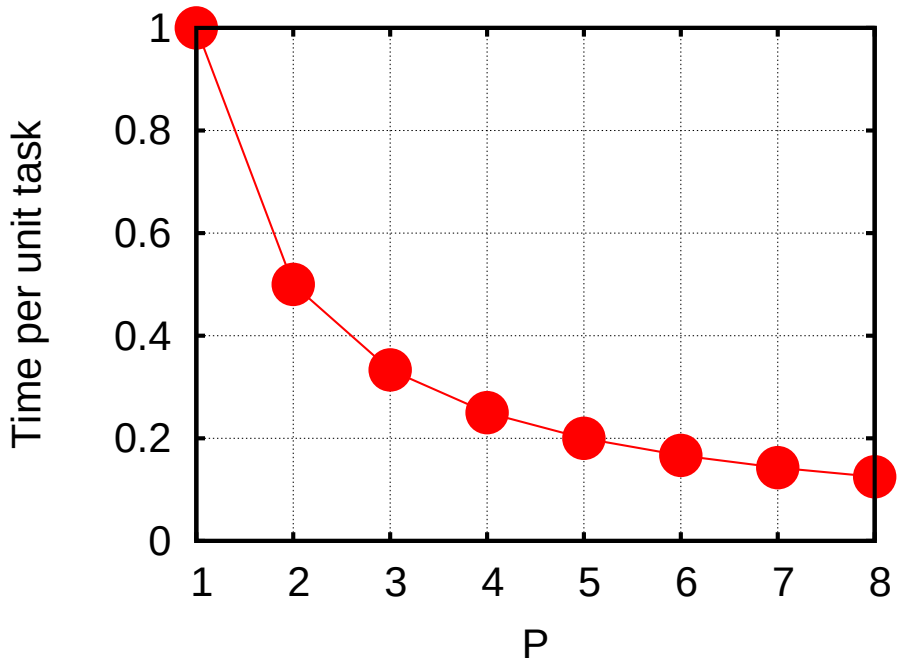


Scaling – Time

- How a problem's timing scales as processor number increases.
- Measured by the time to do one unit. In this case, inverse linear scaling:

$$T \propto 1/P$$

- Again this is the ideal case, or "embarrassingly parallel".



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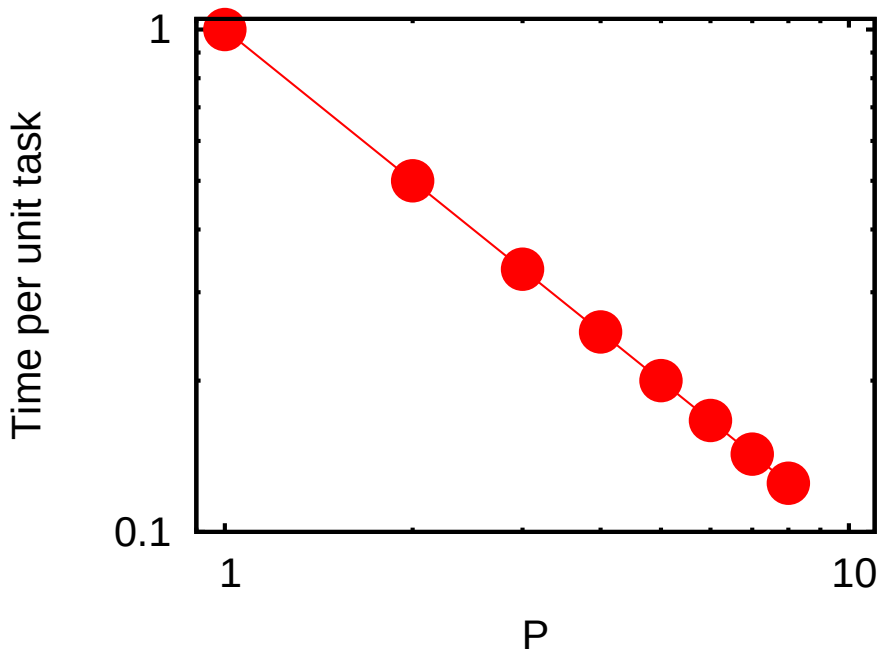
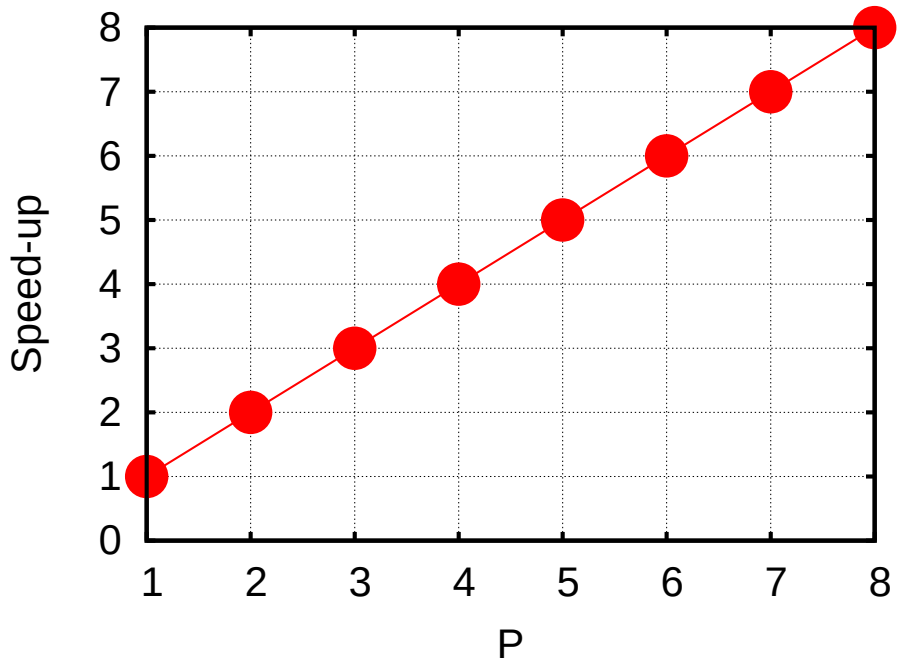


Scaling – Speedup

- How much faster the problem is solved as processor number increases.
- Measured by the serial time divided by the parallel time

$$S = \frac{T_{serial}}{T(P)} \propto P$$

- For embarrassingly parallel applications: Linear speed up.



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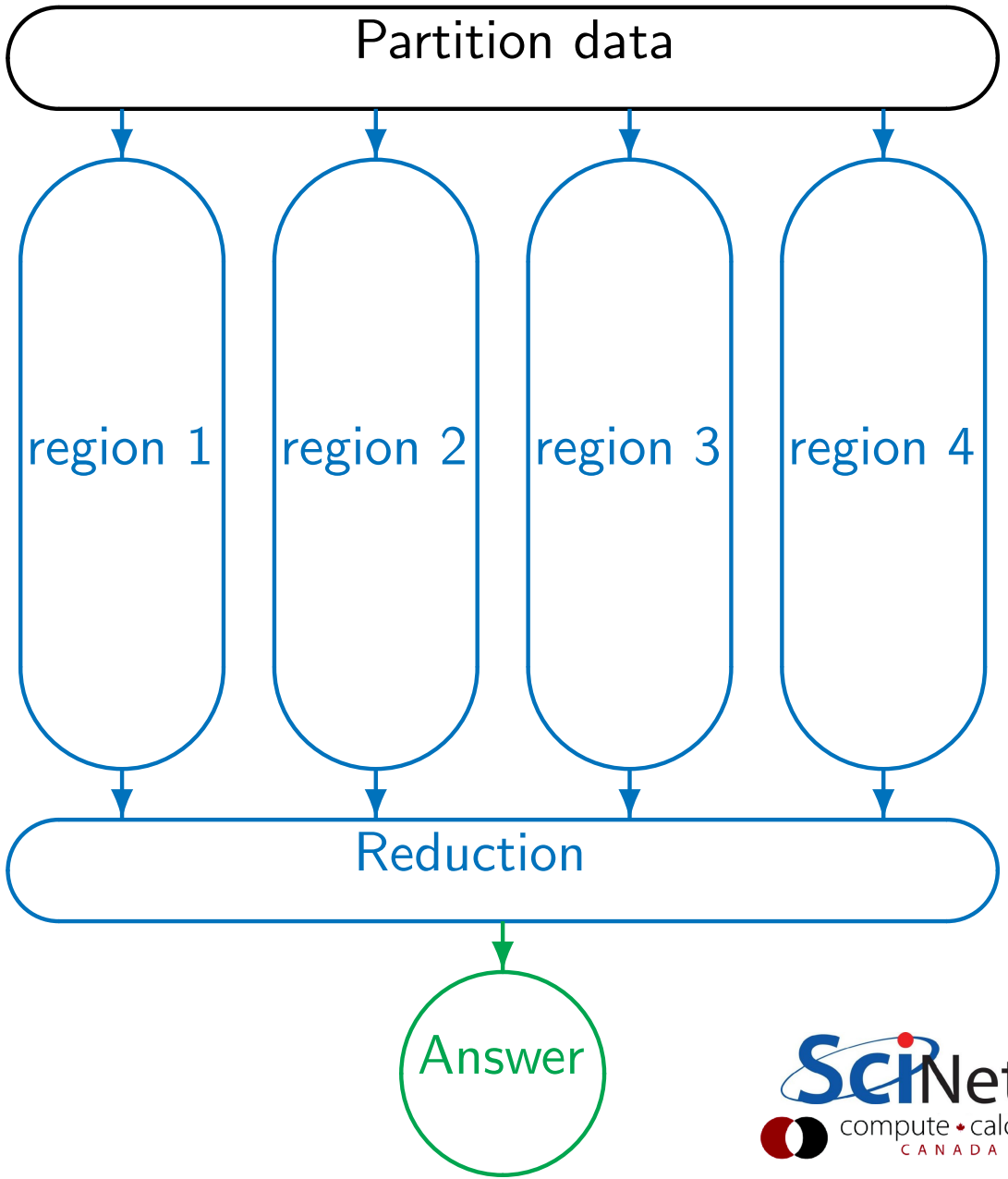
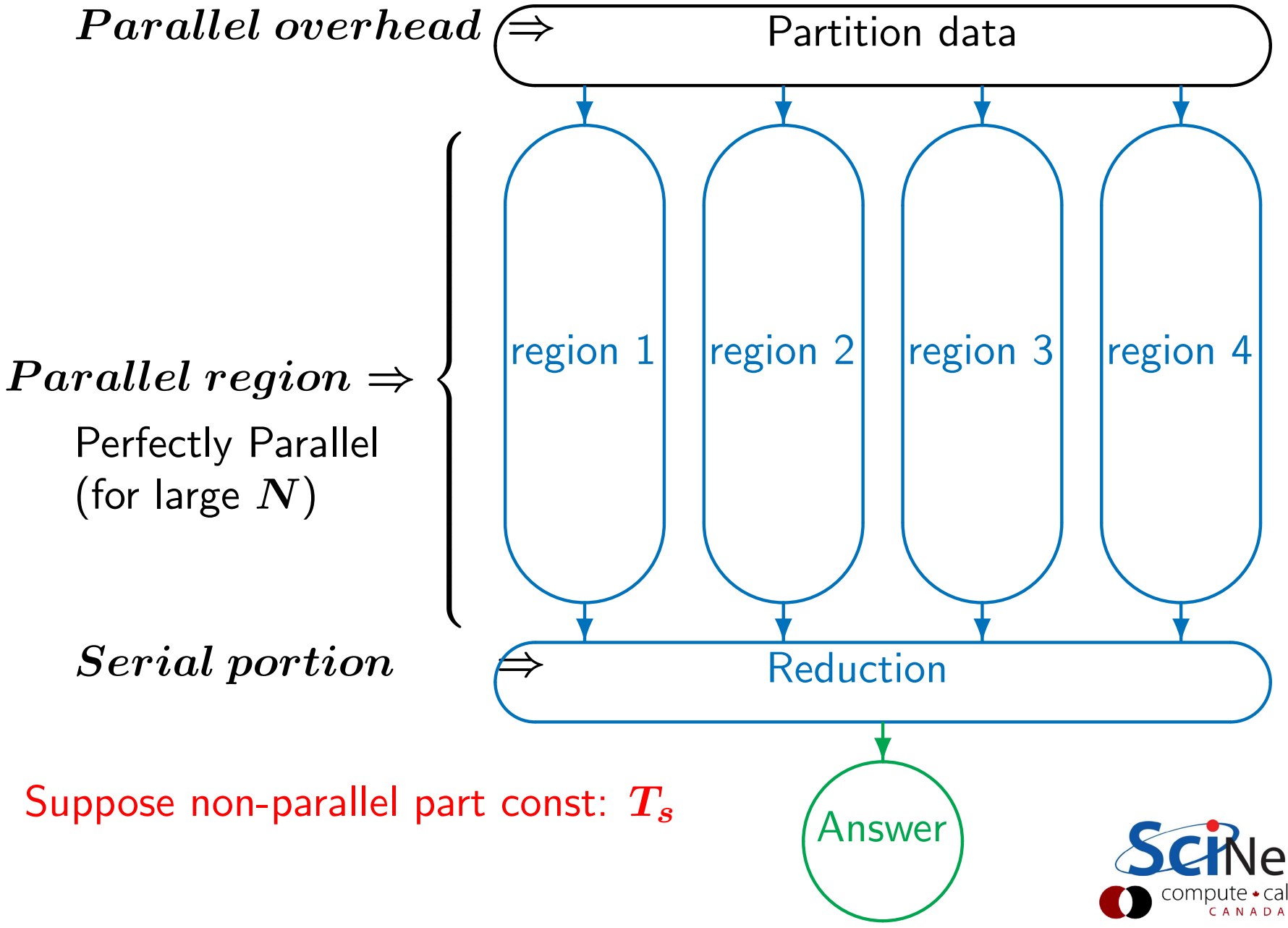
Non-ideal cases

- Say we want to integrate some tabulated experimental data.
- Integration can be split up, so different regions are summed by each processor.
- Non-ideal:
  - First need to get data to processor
  - And at the end bring together all the sums: "reduction"



Non-ideal cases



Suppose non-parallel part const: T_s

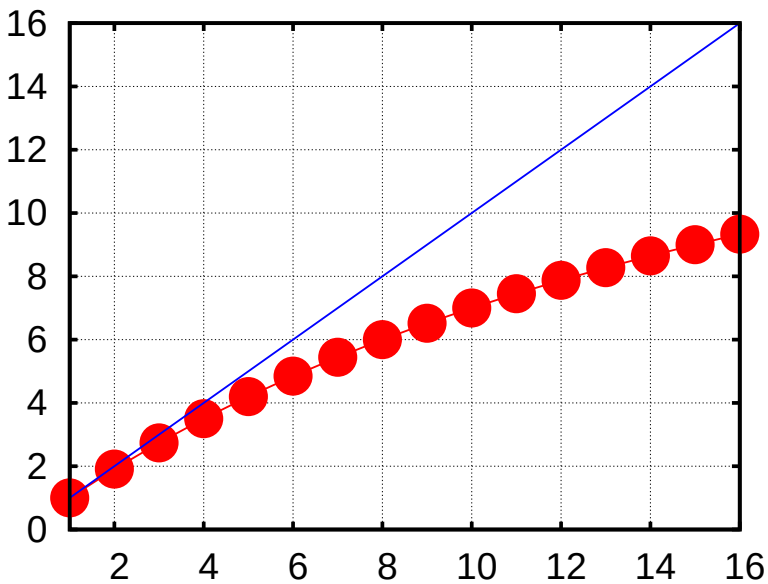
Amdahl's law

Speed-up (without parallel overhead):

$$S = \frac{T_p + T_s}{T_p/P + T_s} = \frac{NT_1 + T_s}{NT_1/P + T_s}$$

or, calling $f = T_s/(T_s + NT_1)$ the serial fraction,

$$S = \frac{1}{f + (1-f)/P}$$



(for $f = 5\%$)

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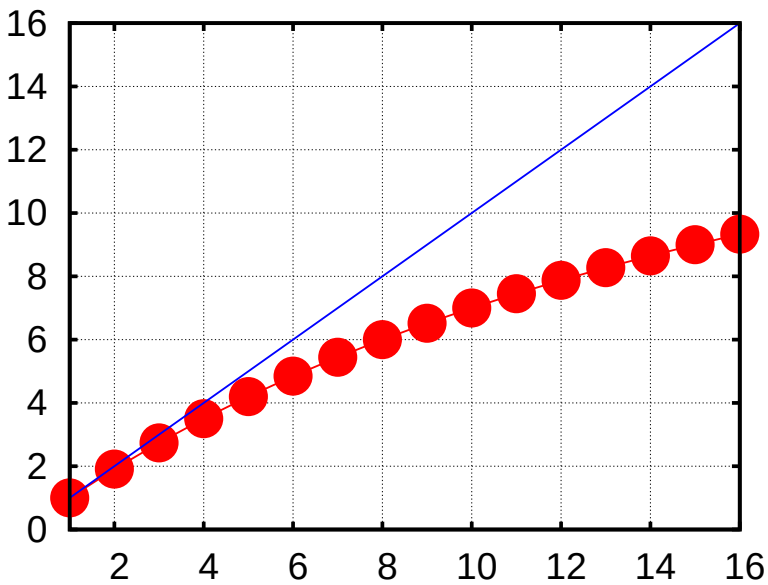

Serial part dominates asymptotically.

Speed-up limited, no matter size of P.

And this is the overly optimistic case!

(for $f = 5\%$)

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HPC Lesson #1

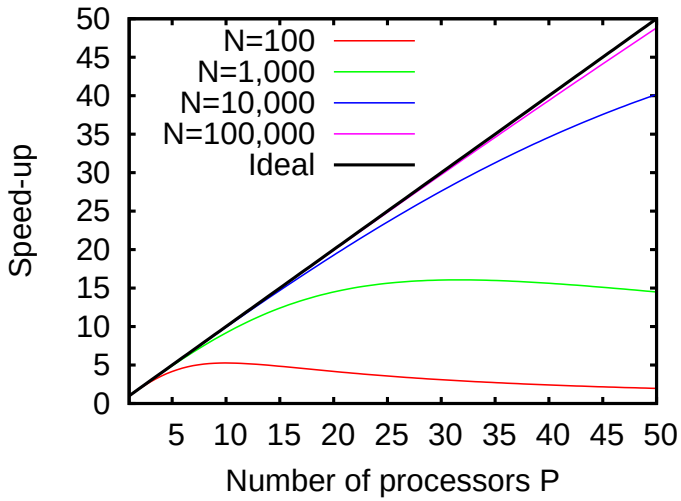
Always keep **throughput** in mind: if you have several runs, running more of them at the same time on fewer processors per run is often advantageous.

Trying to beat Amdahl's law #1

Scale up!

The larger N, the smaller the serial fraction:

$$f(P) = \frac{P}{N}$$



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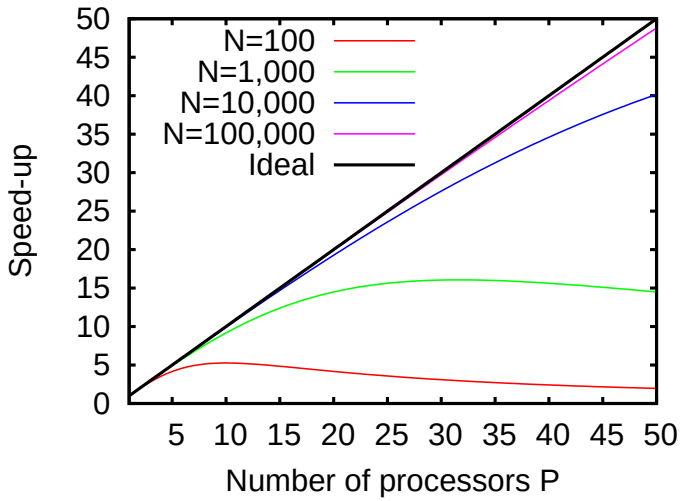

Weak scaling: Increase problem size while increasing P

$$Time_{weak}(P) = Time(N = n \times P, P)$$

Good weak scaling means this time approaches a constant for large P.

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Trying to beat Amdahl's law #1

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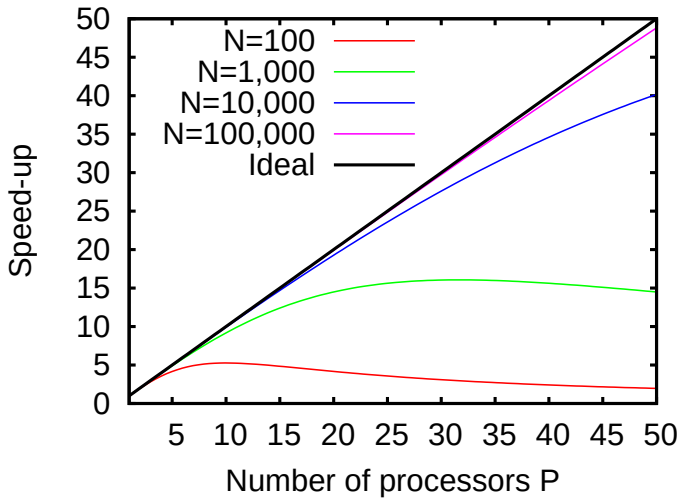

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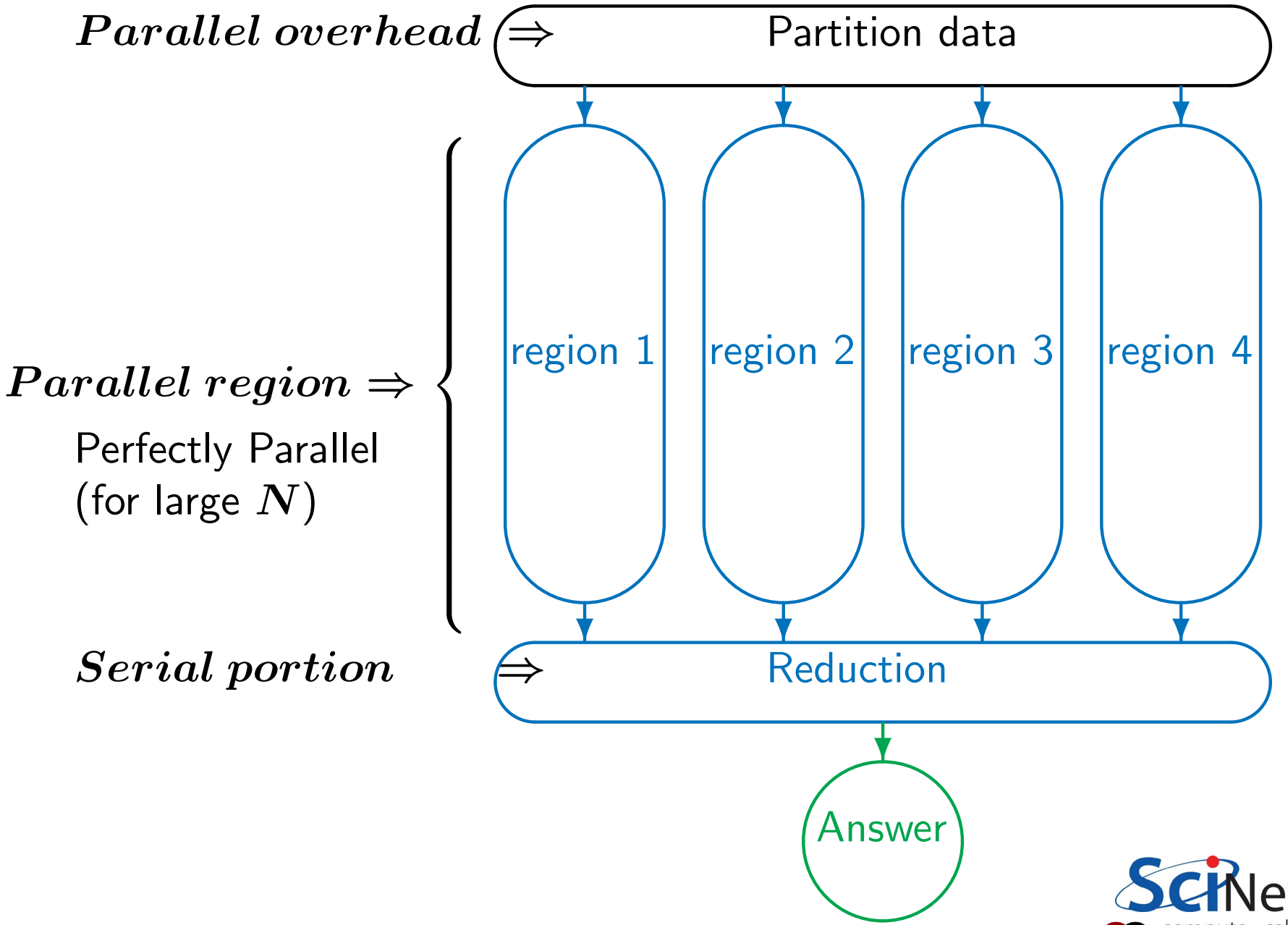
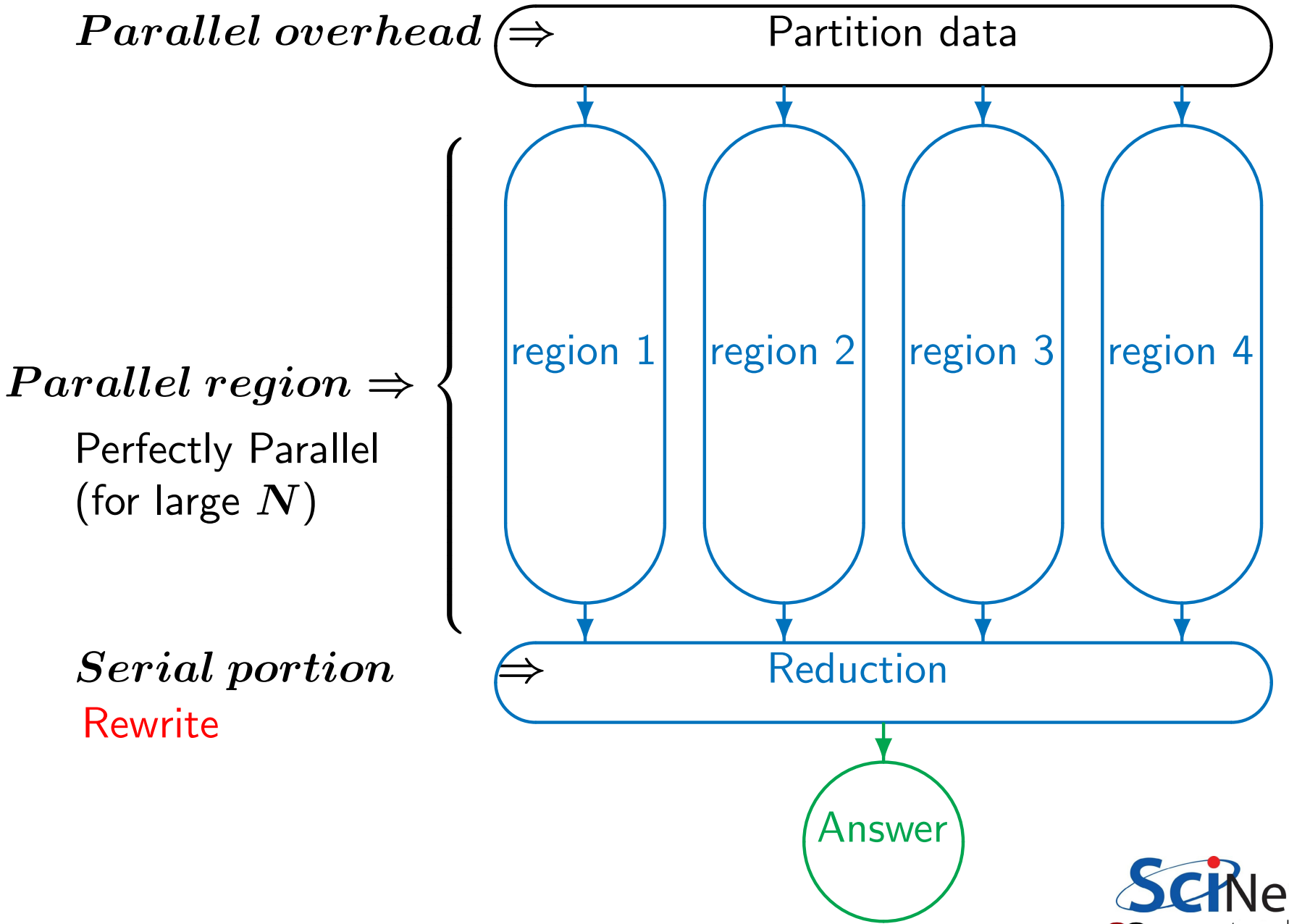
Gustafson's Law

Many large problems can be efficiently parallelized, because N is effectively unbounded.

Trying to beat Amdahl's law #2



Trying to beat Amdahl's law #2



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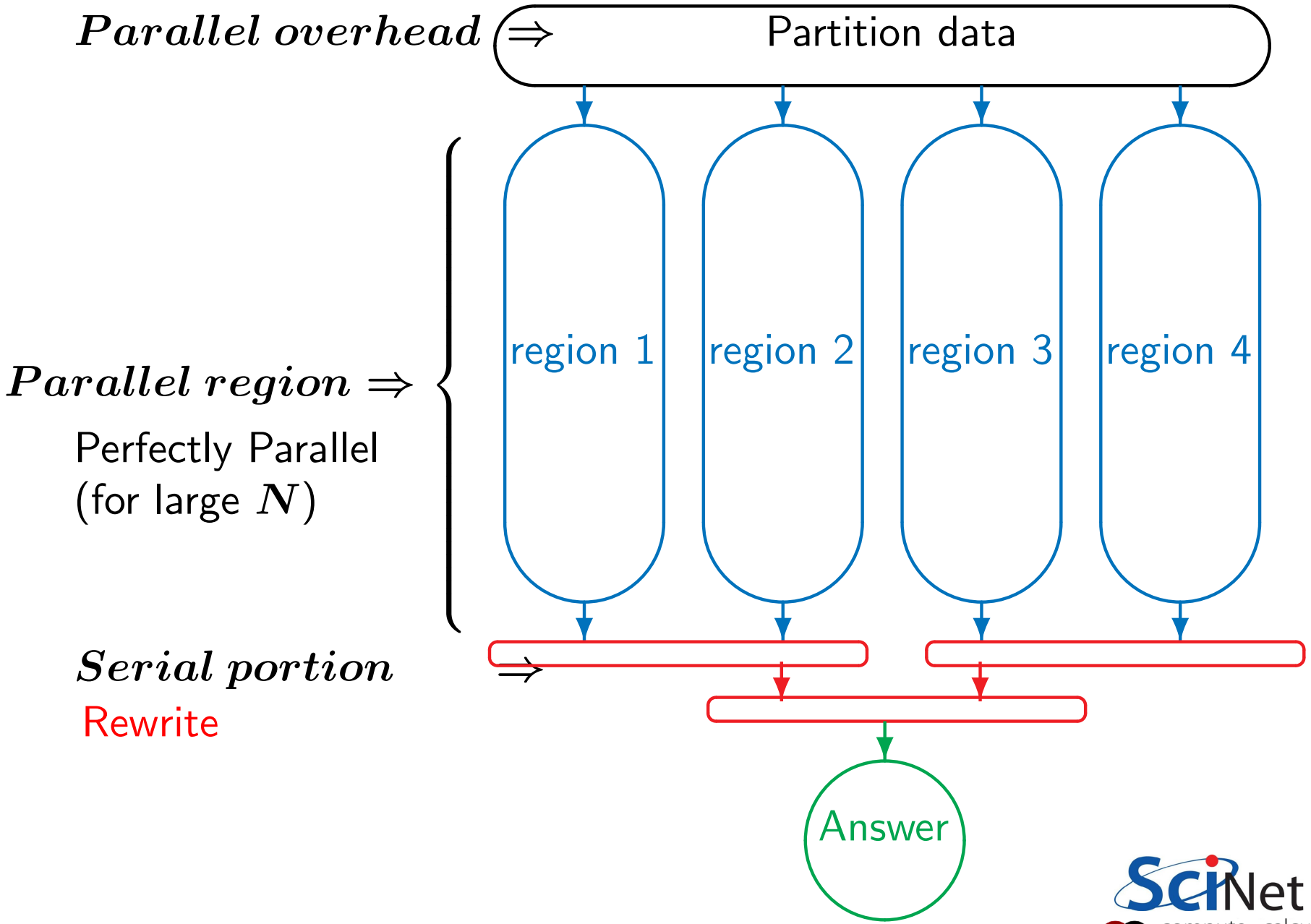
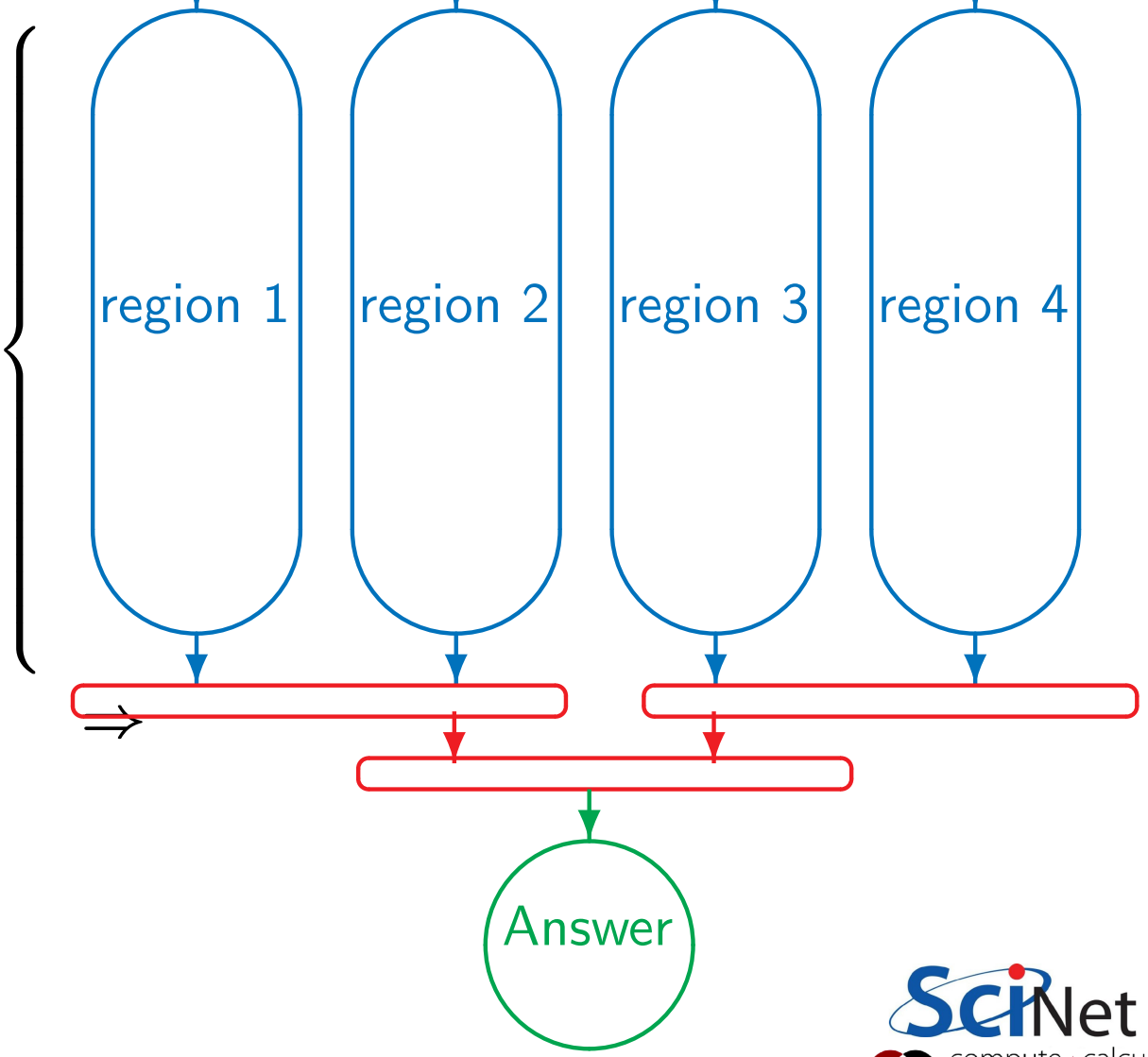


Trying to beat Amdahl's law #2

Parallel overhead $\Rightarrow$ Partition data

Parallel region $\Rightarrow$

Perfectly Parallel
(for large N)



Serial portion $\Rightarrow$

Rewrite

$\propto \log_2(P)$

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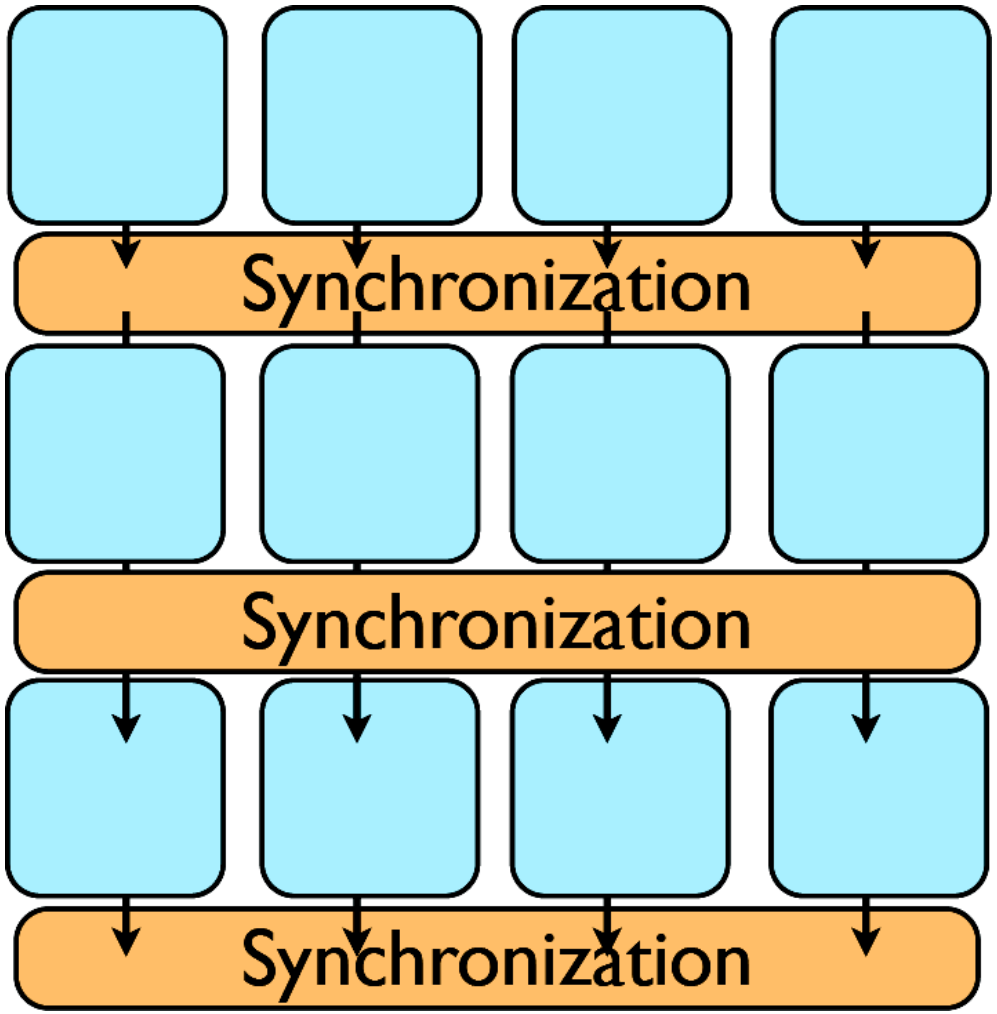
HPC Lesson #2

Optimal Serial Algorithm for your problem may not be the P $\rightarrow$1 limit of your optimal parallel algorithm.

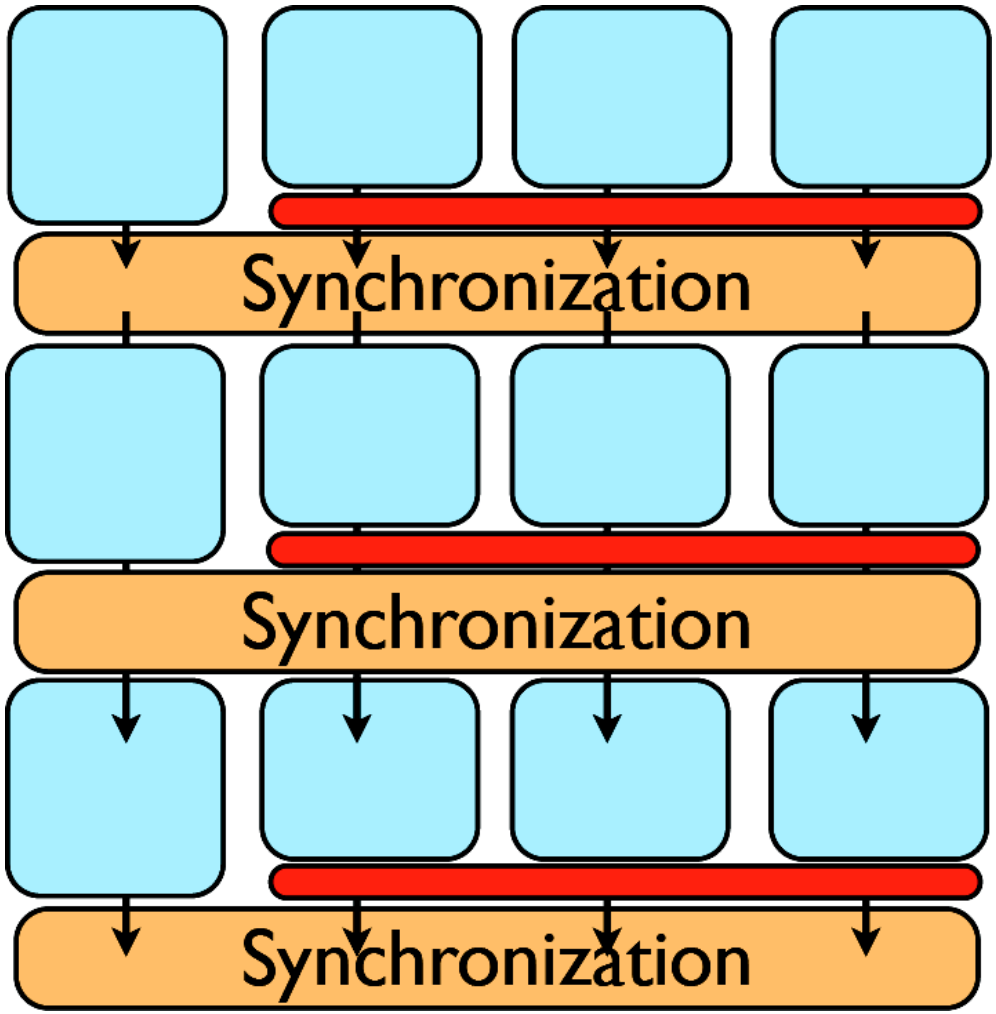
Synchronization

- Most problems are not purely concurrent.
- Some level of synchronization or exchange of information is needed between tasks.
- While synchronizing, nothing else happens: increases Amdahl's f.
- And synchronizations are themselves costly.



Load Balancing

- The division of calculations among the processors may not be equal.
- Some processors would already be done, while others are still going.
- Effectively using less than P processors: This reduces the efficiency.
- Aim for load balanced algorithms.



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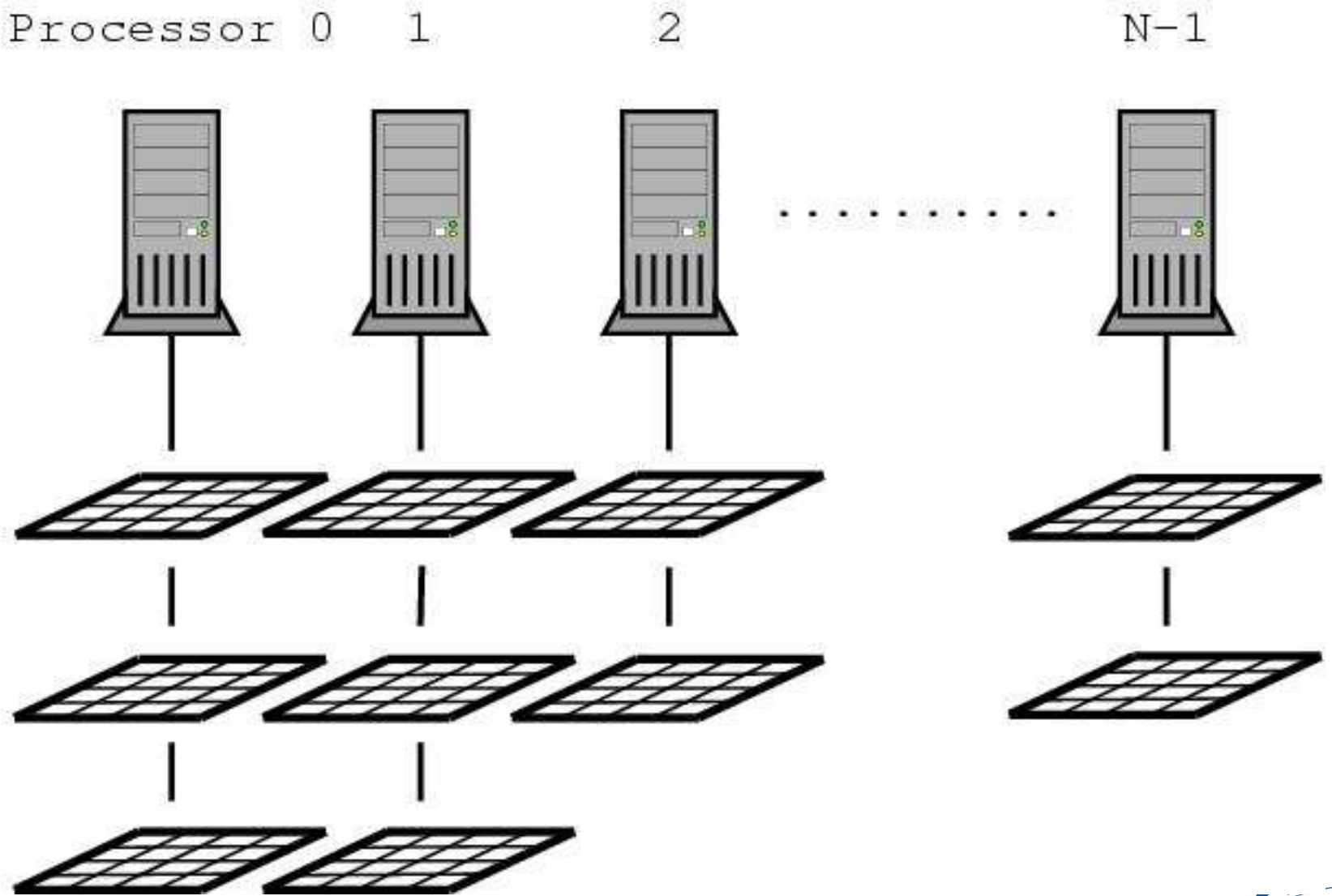
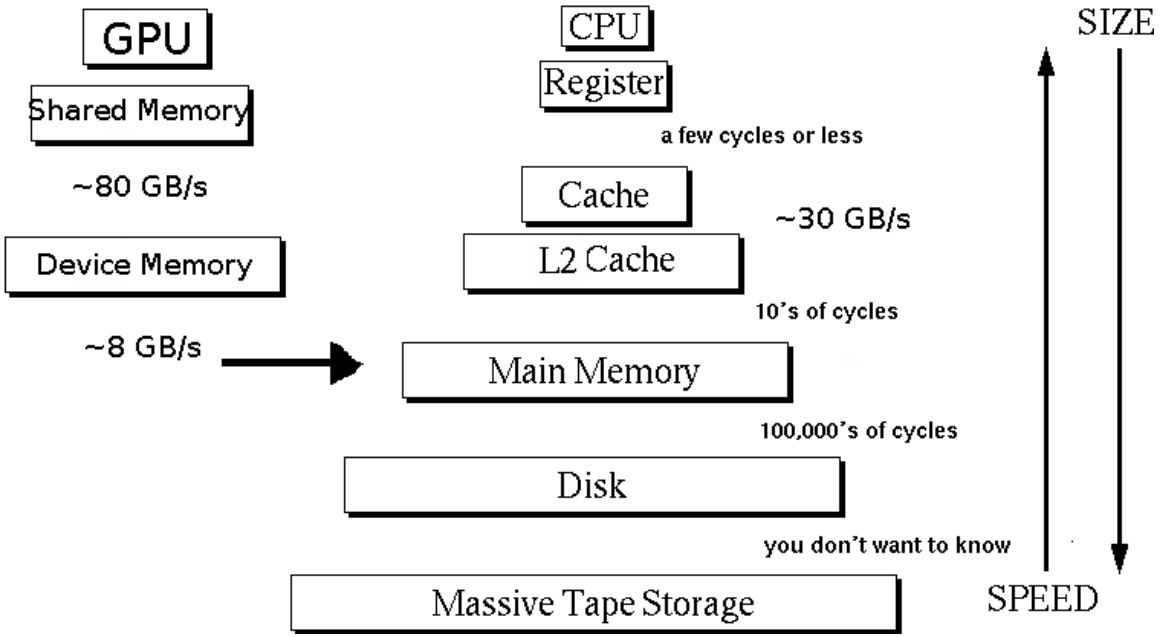
Load Balancing



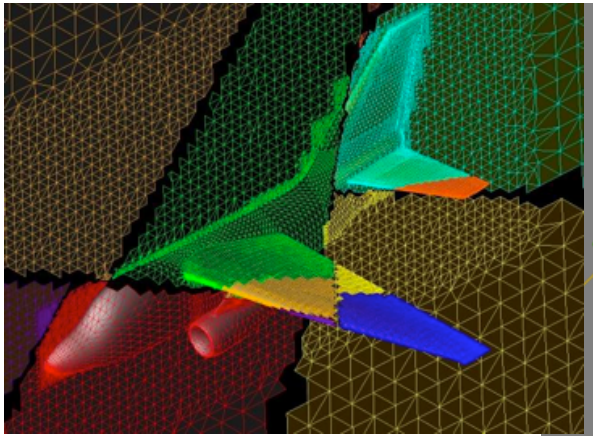
Locality

- So far we neglected communication costs.
- But communication costs are more expensive than computation!
- To minimize communication to computation ratio:
  * Keep the data where it is needed.
  * Make sure as little data as possible is to be communicated.
  * Make shared data as local to the right processors as possible.
- Local data means less need for syncs, or smaller-scale syncs.
- Local syncs can alleviate load balancing issues.

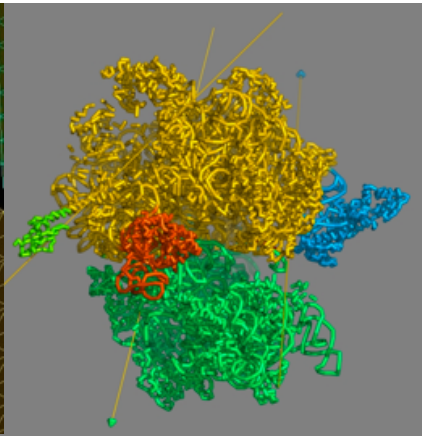
Locality


GPU
Shared Memory
~80 GB/s
Device Memory
~8 GB/s
CPU
Register
a few cycles or less
Cache
~30 GB/s
L2 Cache
10's of cycles
Main Memory
100,000's of cycles
Disk
you don't want to know
Massive Tape Storage
SIZE
SPEED

Domain Decomposition



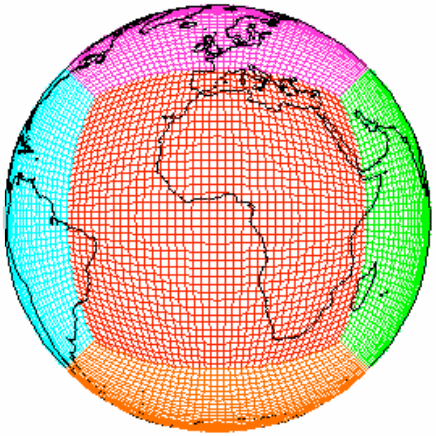
http://adg.stanford.edu/aa241/design/compaero.html



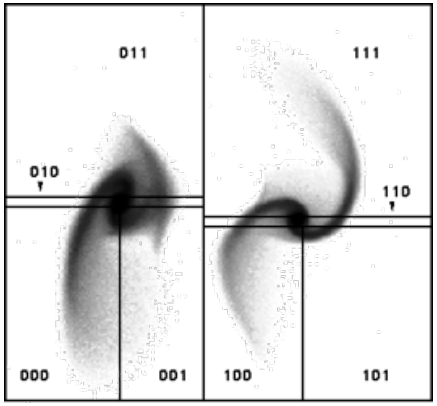
http://www.uea.ac.uk/cmp/research/cmpbio/Protein+Dynamics,+Structure+and+Function

Domain Decomposition

- A very common approach to parallelizing on distributed memory computers
- Maintain Locality; need local data mostly, this means only surface data needs to be sent between processes.



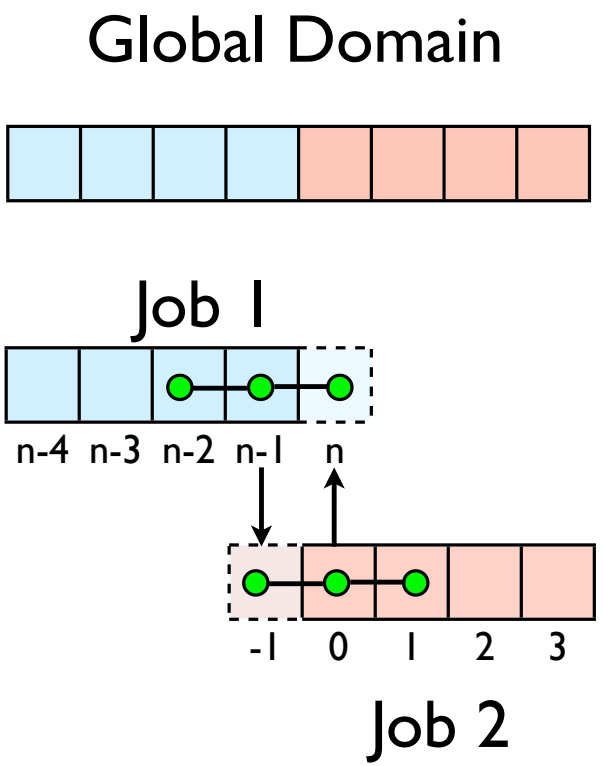
http://sivo.gsfc.nasa.gov/cubedsphere_comp.html



http://www.cita.utoronto.ca/~dubinski/treecode/node8.html

Guardcells

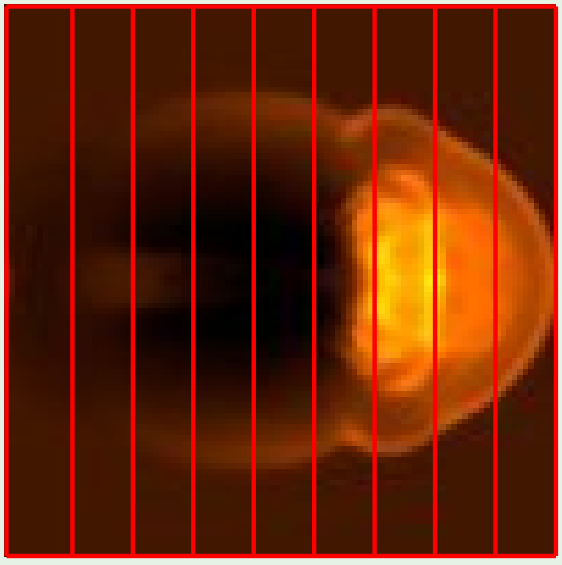
- Works for parallel decomposition!
- Job 1 needs info on Job 2s 0th zone, Job 2 needs info on Job 1s last zone
- Pad array with 'guardcells' and fill them with the info from the appropriate node by message passing or shared memory



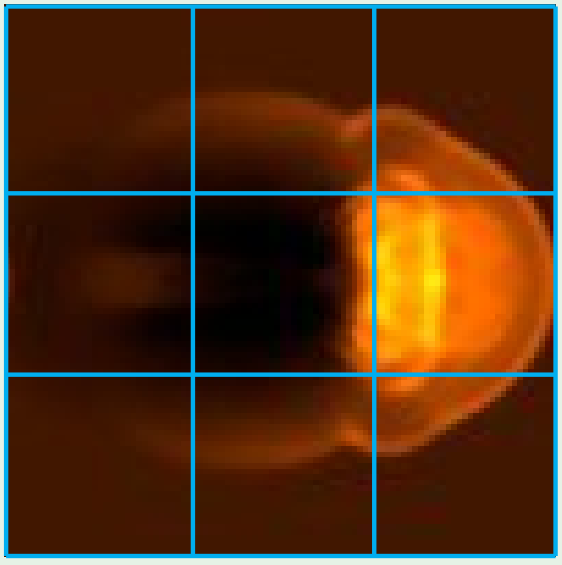
Locality

Example (PDE Domain decomposition)

wrong



right



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HPC Lesson #3

Parallel algorithm design is about finding as much **concurrency** as possible, and arranging it in a way that maximizes **locality**.

Outline

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HPC Systems

Top500.org:

List of the worlds 500 largest supercomputers. Updated every 6 months,

Info on architecture, etc.

Top500 List - November 2013

R_{max} and R_{peak} values are in TFlops. For more details about other fields, check the TOP500 description.

R_{peak} values are for the normal CPU clock rate. For the effeciency of the systems you should take the Turbu CPU clock rate into account.

previous | 1 | 2 | 3 | 4 | 5 | next

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3120000	33862.7	54902.4	17808
2	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560640	17590.0	27112.5	8209
3	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1572864	17173.2	20132.7	7890
4	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705024	10510.0	11280.4	12660
5	DOE/SC/Argonne National Laboratory United States	**Mira** - BlueGene/Q, Power BQC 16C 1.60GHz, Custom IBM	786432	8586.6	10066.3	3945
6	Swiss National Supercomputing Centre (CSCS) Switzerland	**Piz Daint** - Cray XC30, Xeon E5-2670 8C 2.600GHz, Aries interconnect , NVIDIA K20x Cray Inc.	115984	6271.0	7788.9	2325
7	Texas Advanced Computing Center/Univ. of Texas United States	**Stampede** - PowerEdge C8220, Xeon E5-2680 8C 2.700GHz, Infiniband FDR, Intel Xeon Phi SE10P Dell	462462	5168.1	8520.1	4510
8	Forschungszentrum Juelich (FZJ) Germany	**JUQUEEN** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	458752	5008.9	5872.0	2301
9	DOE/NNSA/LLNL United States	**Vulcan** - BlueGene/Q, Power BQC 16C 1.600GHz, Custom Interconnect IBM	393216	4293.3	5033.2	1972
10	Leibniz Rechenzentrum Germany	**SuperMUC** - iDataPlex DX360M4, Xeon E5-2680 8C 2.70GHz, Infiniband FDR IBM	147456	2897.0	3185.1	3423

HPC Systems

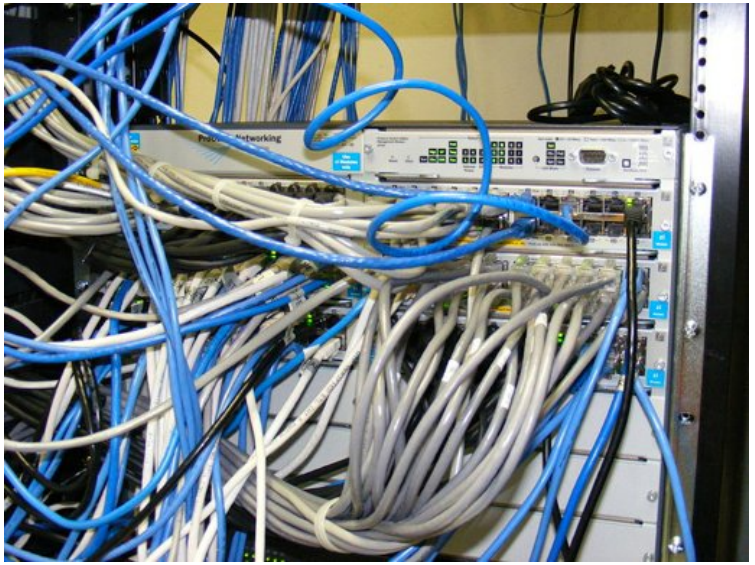
Architectures

- Clusters, or, distributed memory machines
  - A bunch of servers linked together by a network ("interconnect").
  - commodity x86 with gigE, Cray XK, IBM BGQ
- Symmetric Multiprocessor (SMP) machines, or, shared memory machines
  - These can all see the same memory, typically a limited number of cores.
  - IBM Pseries, Cray SMT, SGI Altix/UV
- Vector machines.
  - No longer dominant in HPC anymore.
  - Cray, NEC
- Accelerator (GPU, KNL, FPGA)
  - Heterogeneous use of standard CPU's with a specialized accelerator.
  - NVIDIA, AMD, Xilinx, Altera

Distributed Memory: Clusters

Simplest type of parallel computer to build

- Take existing powerful standalone computers
- And network them



(source: http://flickr.com/photos/eurleif)

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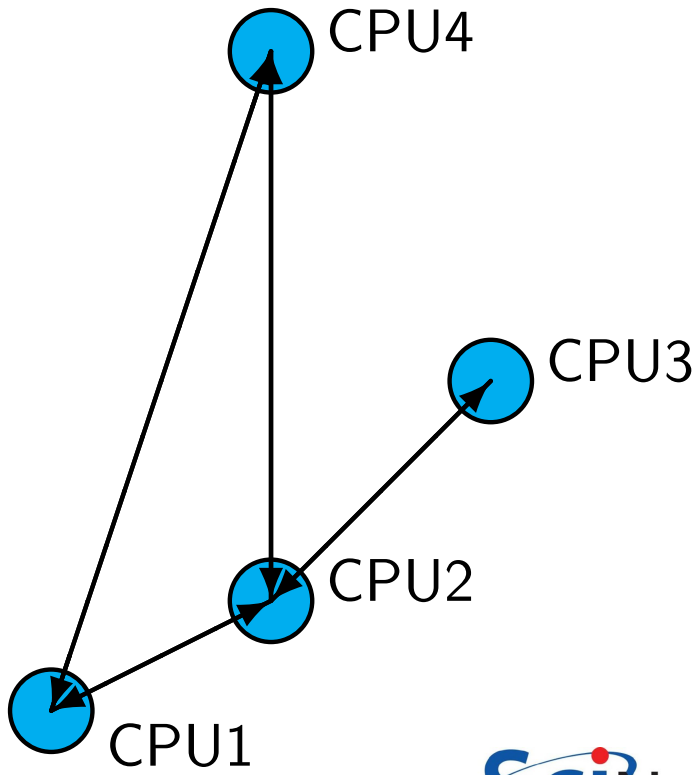
Distributed Memory: Clusters

Each node is independent!

Parallel code consists of programs running on separate computers, communicating with each other.

Could be entirely different programs.



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Distributed Memory: Clusters

Each node is independent!

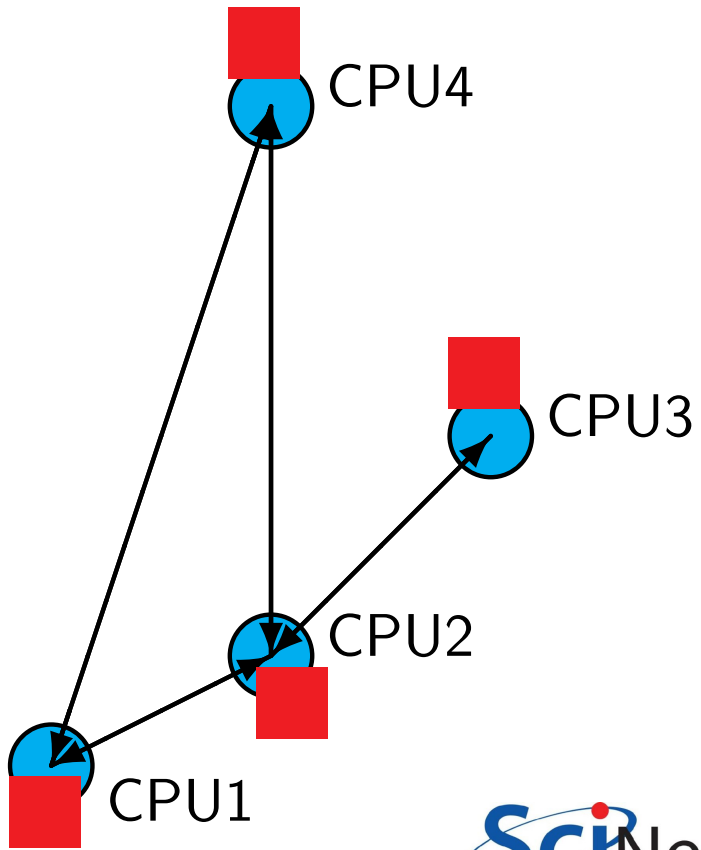
Parallel code consists of programs running on separate computers, communicating with each other.

Could be entirely different programs.

Each node has own memory!

Whenever it needs data from another region, requests it from that CPU.

Usual model: "message passing"



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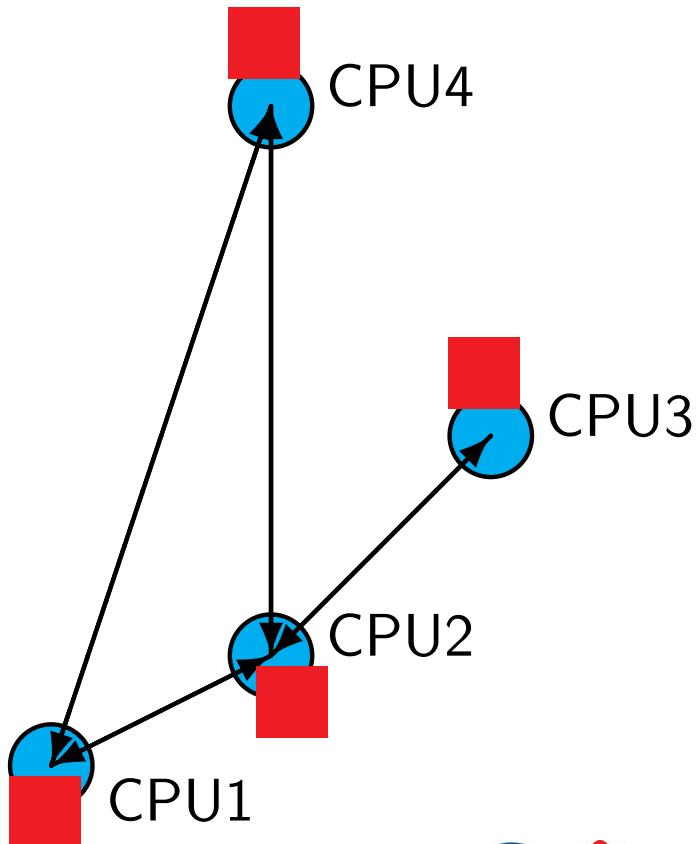
Clusters+Message Passing

Hardware:

Easy to build
(Harder to build well)
Can build larger and
larger clusters relatively
easily

Software:

Every communication
has to be hand-coded:
hard to program



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Task (function, control) Parallelism

Work to be done is decomposed across processors

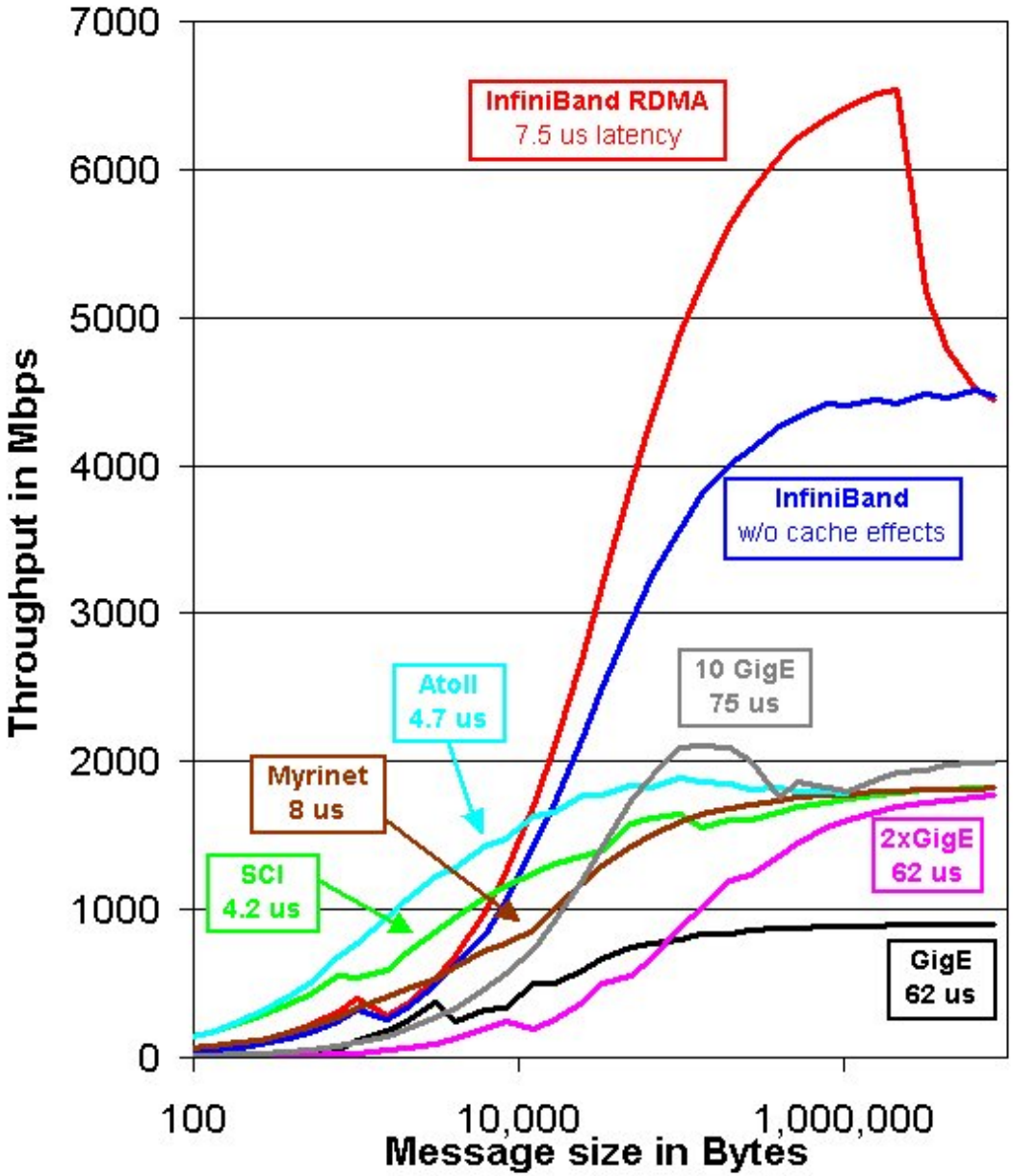
- e.g. divide and conquer
- each processor responsible for some part of the algorithm
- communication mechanism is significant
- must be possible for different processors to be performing different tasks

Cluster Communication Cost

	Latency	Bandwidth
GigE	10 μs (10,000 ns)	1 Gb/s (60 ns/double)
Infiniband	2 μs (2,000 ns)	2-10 Gb/s (10 ns /double)

Processor speed: O(GFLOP) $\sim$ few ns or less.

Cluster Communication Cost



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SciNet Niagara Cluster

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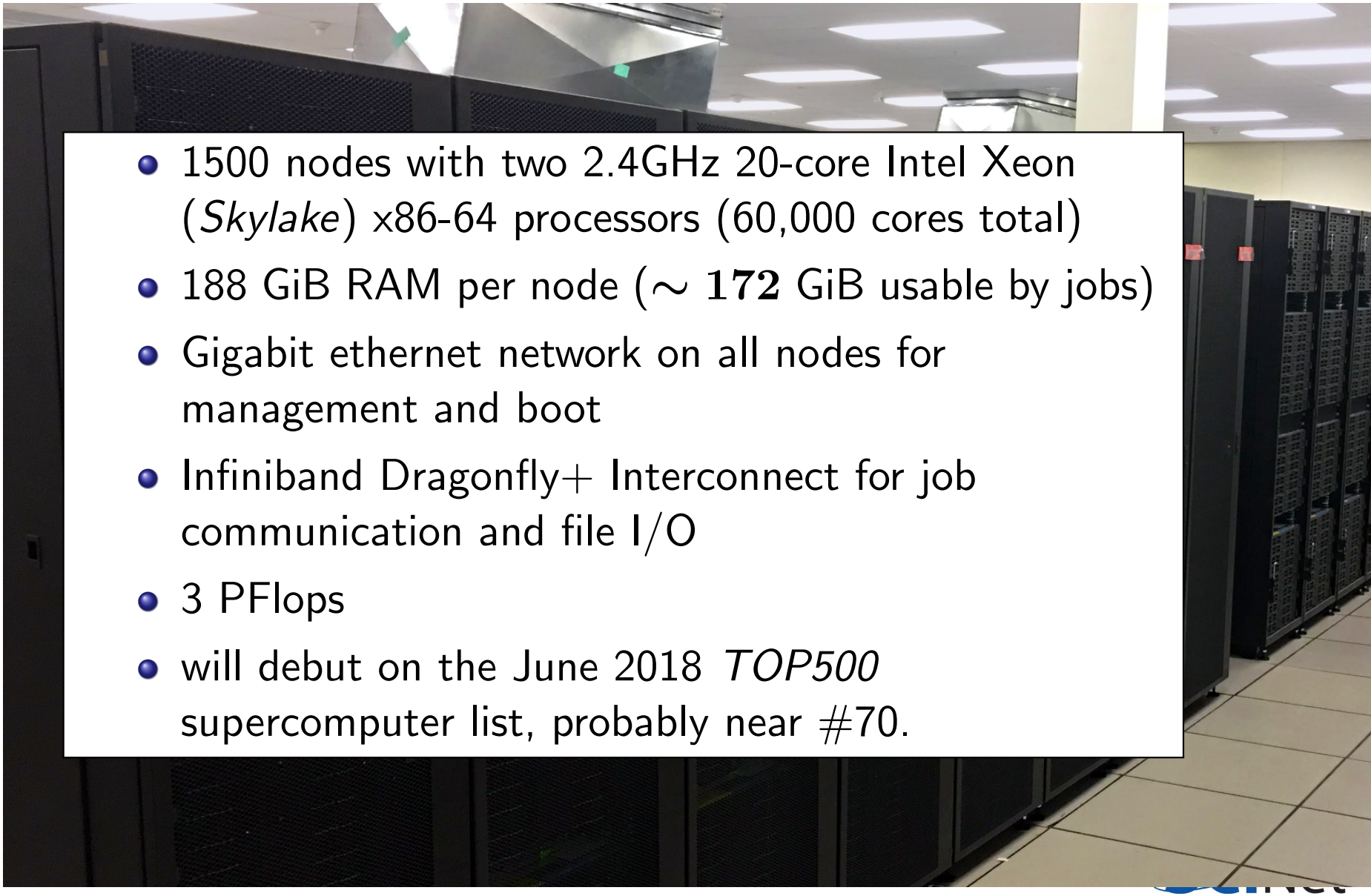
SciNet Niagara Cluster



- 1500 nodes with two 2.4GHz 20-core Intel Xeon (*Skylake*) x86-64 processors (60,000 cores total)
- 188 GiB RAM per node ($\sim$ **172** GiB usable by jobs)
- Gigabit ethernet network on all nodes for management and boot
- Infiniband Dragonfly+ Interconnect for job communication and file I/O
- 3 PFlops
- will debut on the June 2018 *TOP500* supercomputer list, probably near #70.

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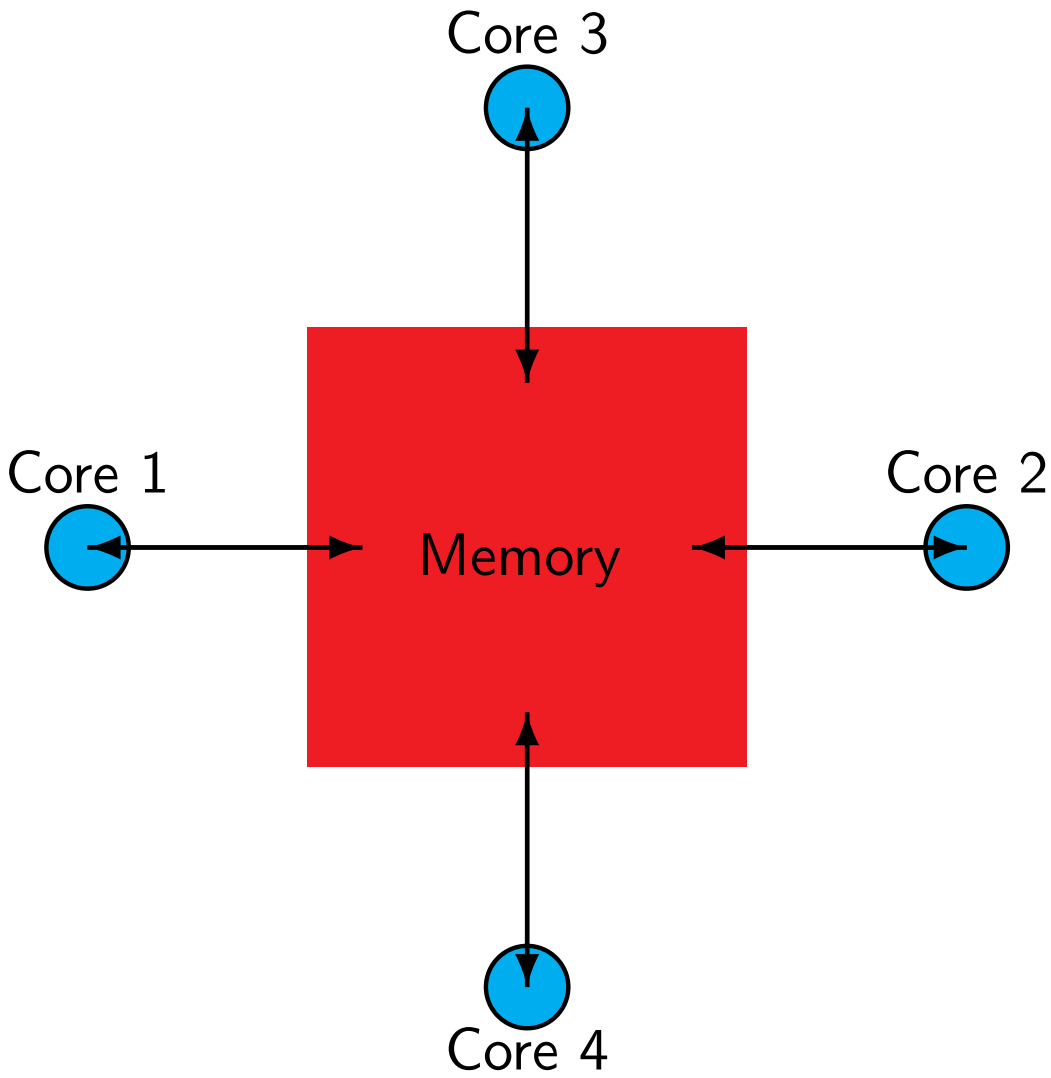
Shared Memory

One large bank of memory, different computing cores acting on it. All 'see' same data.

Any coordination done through memory

Could use message passing, but no need.

Each core is assigned a thread of execution of a single program that acts on the data.



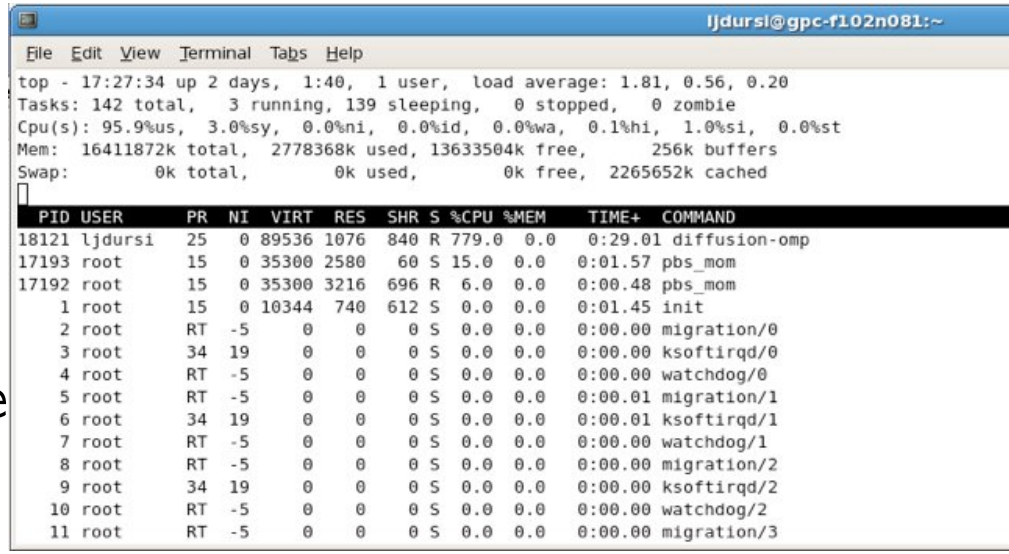
Threads versus Processes

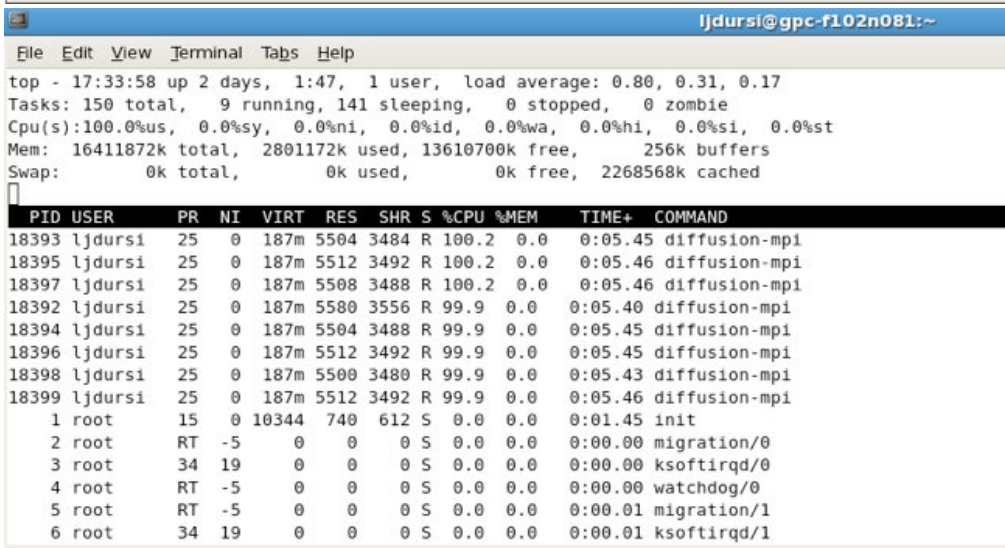
Threads:

Threads of execution within one process, with access to the same memory etc.

Processes:

Independent tasks with their own memory and resources





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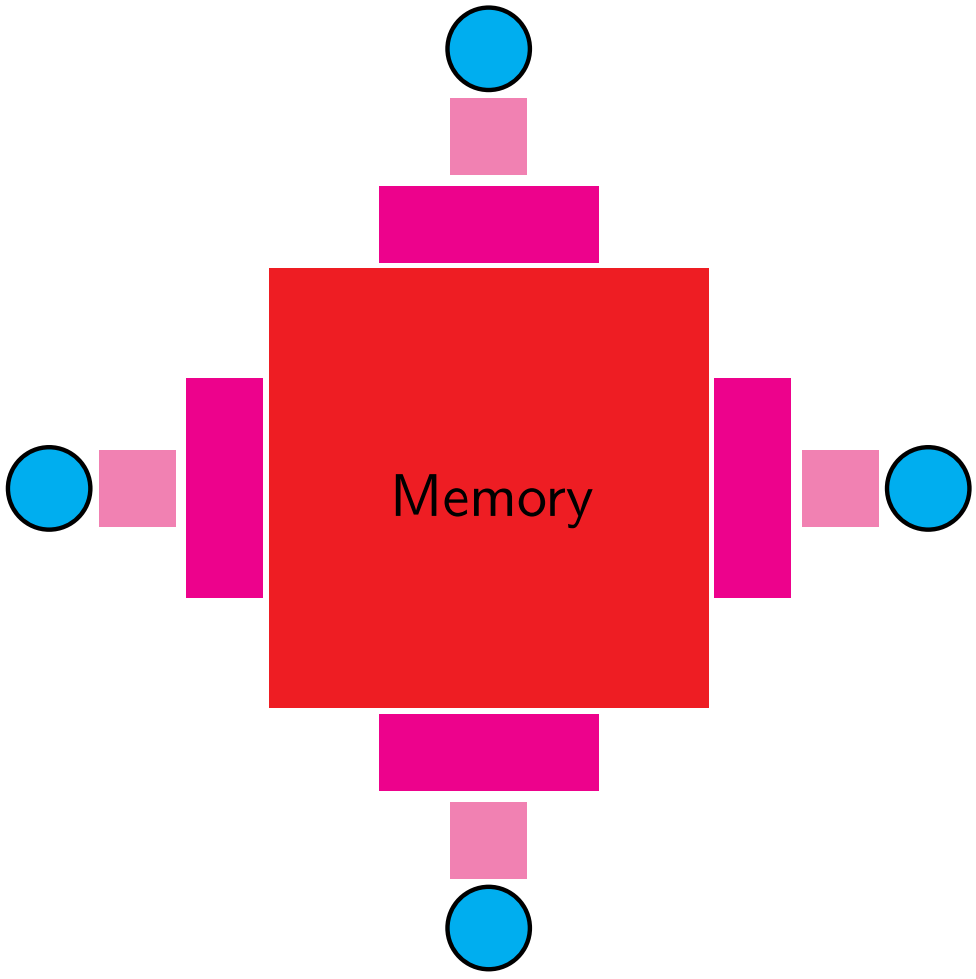
Shared Memory: NUMA

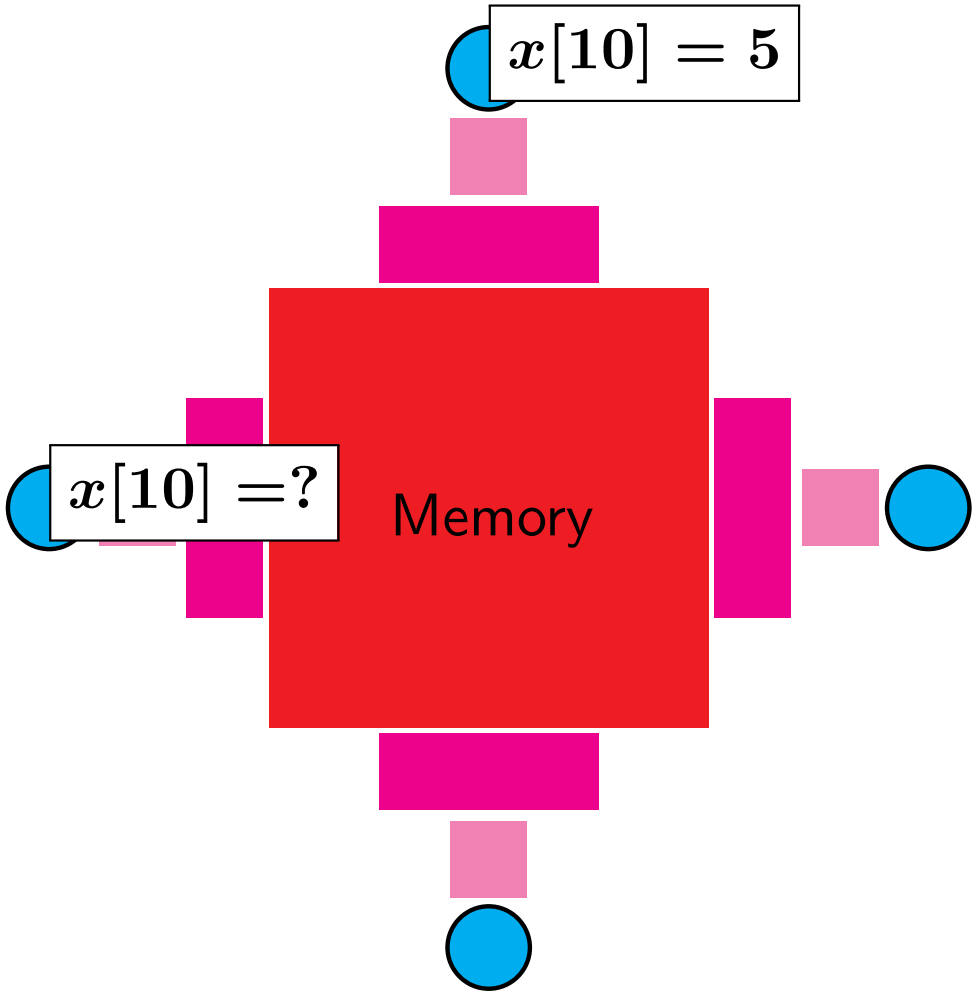
Non-Uniform Memory Access

- Each core typically has some memory of its own.
- Cores have cache too.
- Keeping this memory coherent is extremely challenging.



Coherency

- The different levels of memory imply multiple copies of some regions
- Multiple cores mean can update unpredictably
- Very expensive hardware
- Hard to scale up to lots of processors.
- Very simple to program!!



Data (Loop) Parallelism

Data is distributed across processors

- easier to program, compiler optimization
- code otherwise looks fairly sequential
- benefits from minimal communication overhead
- scale limitations

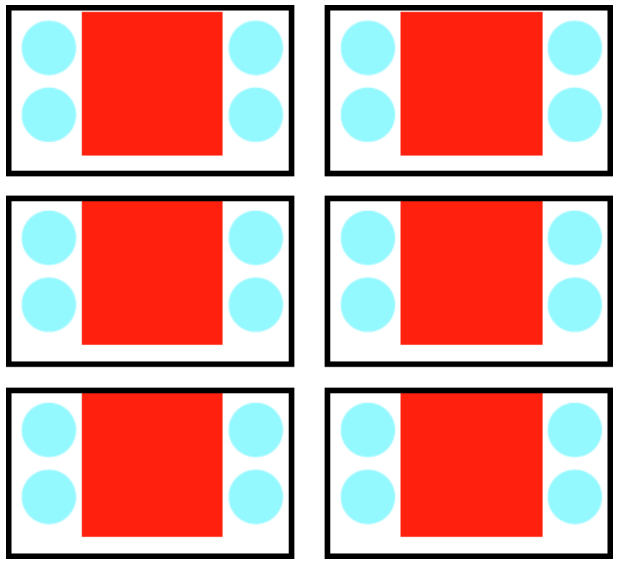
Shared Memory Communication Cost

	Latency	Bandwidth
GigE	10 μs (10,000 ns)	1 Gb/s (60 ns/double)
Infiniband	2 μs (2,000 ns)	2-10 Gb/s (10 ns /double)
NUMA (shared memory)	0.1 μs (100 ns)	10-20 Gb/s (4 ns /double)

Processor speed: O(GFLOP) $\sim$ few ns or less.

Hybrid Architectures

- Use shared and distributed memory together (i.e. OpenMP with MPI).
- Need to exploit multi-level parallelism.
- Homogeneous
  - Identical multicore machines linked together with an interconnect.
  - Many cores have modest vector capabilities.
  - Thread on-node, MPI for off-node.
- Heterogeneous
  - Same as above, but with an accelerator as well.
  - GPU, FPGA.



Heterogeneous Computing

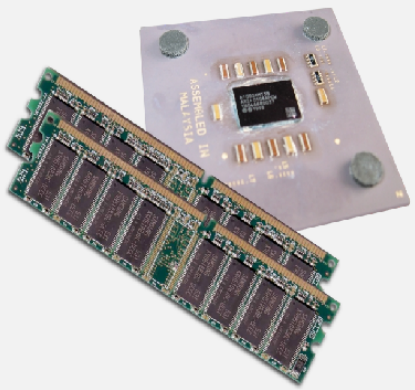
What is it?

- Use different compute device(s) concurrently in the same computation.
- Commonly using a CPU with an accelator: GPU, FPGA, ...
- Example: Leverage CPUs for general computing components and use GPU's for data parallel / FLOP intensive components.
- Pros: Faster and cheaper ($/FLOP/Watt) computation
- Cons: More complicated to program

Heterogeneous Computing

Terminology

- GPGPU : General Purpose Graphics Processing Unit
- HOST : CPU and its memory
- DEVICE : Accelerator (GPU) and its memory



Host

Device

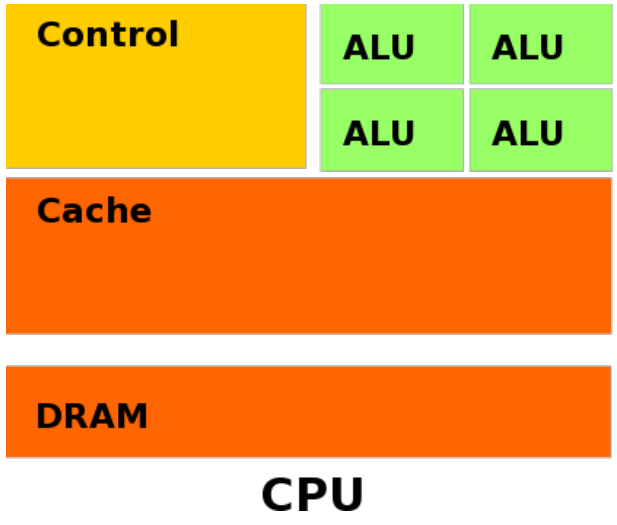
GPU vs. CPUs

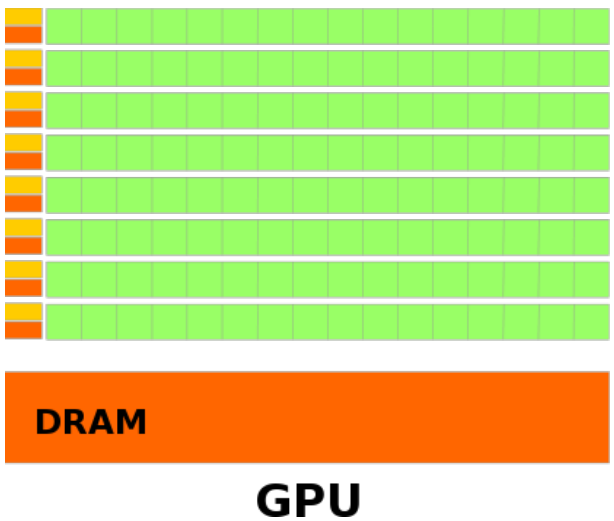
CPU

- general purpose
- task parallelism (diverse tasks)
- maximize serial performance
- large cache
- multi-threaded (4-16)
- some SIMD (SSE, AVX)

GPU

- data parallelism (single task)
- maximize throughput
- small cache
- super-threaded (500-2000+)
- almost all SIMD





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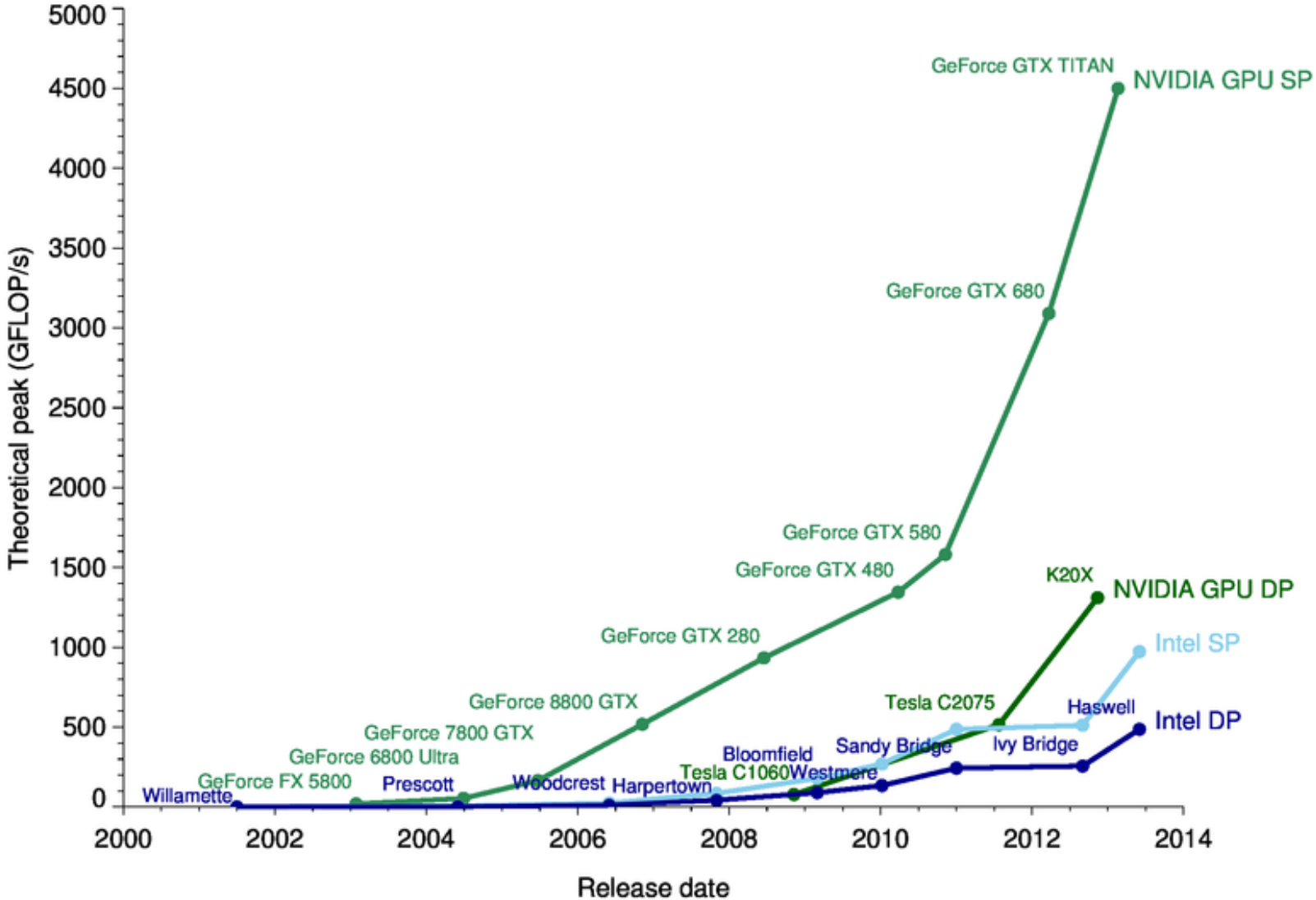
GPGPU



http://michaelgalloy.com/2013/06/11/cpu-vs-gpu-performance.html

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Heterogeneous Speedup

What kind of speedup can I expect?

- ∼1 TFLOPs per GPU vs. ∼100 GFLOPs multi-core CPU
- 0x - 50x reported

Heterogeneous Speedup

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- ∼1 TFLOPs per GPU vs. ∼100 GFLOPs multi-core CPU
- 0x - 50x reported

Speedup depends on

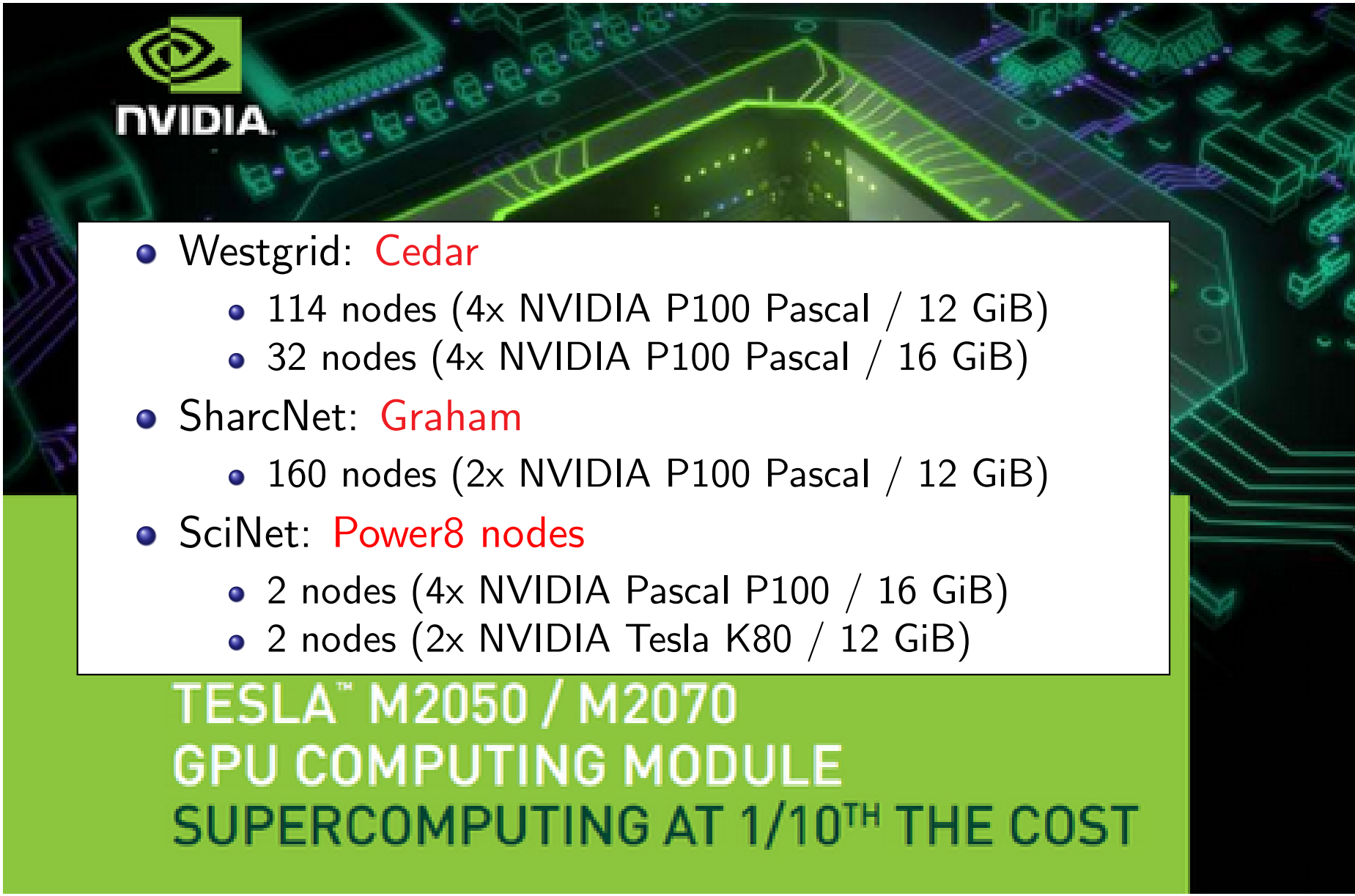
- problem structure
  - need many identical independent calculations
  - preferably sequential memory access
- single vs. double precision (K20 3.52 TF SP vs 1.17 TF DP)
- data locality
- level of intimacy with hardware
- programming time investment

Accelerator Programming

Languages

- GPGPU Only
  - OpenGL, DirectX (Graphics only)
  - CUDA (NVIDIA proprietary)
- OpenCL (1.0, 1.1, 2.0)
- OpenACC
- OpenMP 4.0/4.5

Compute Canada GPU Resources



- Westgrid: Cedar
  - 114 nodes (4x NVIDIA P100 Pascal / 12 GiB)
  - 32 nodes (4x NVIDIA P100 Pascal / 16 GiB)
- SharcNet: Graham
  - 160 nodes (2x NVIDIA P100 Pascal / 12 GiB)
- SciNet: Power8 nodes
  - 2 nodes (4x NVIDIA Pascal P100 / 16 GiB)
  - 2 nodes (2x NVIDIA Tesla K80 / 12 GiB)

HPC Lesson #4

The best approach to parallelizing your problem will depend on both details of your problem and of the hardware available.

Outline

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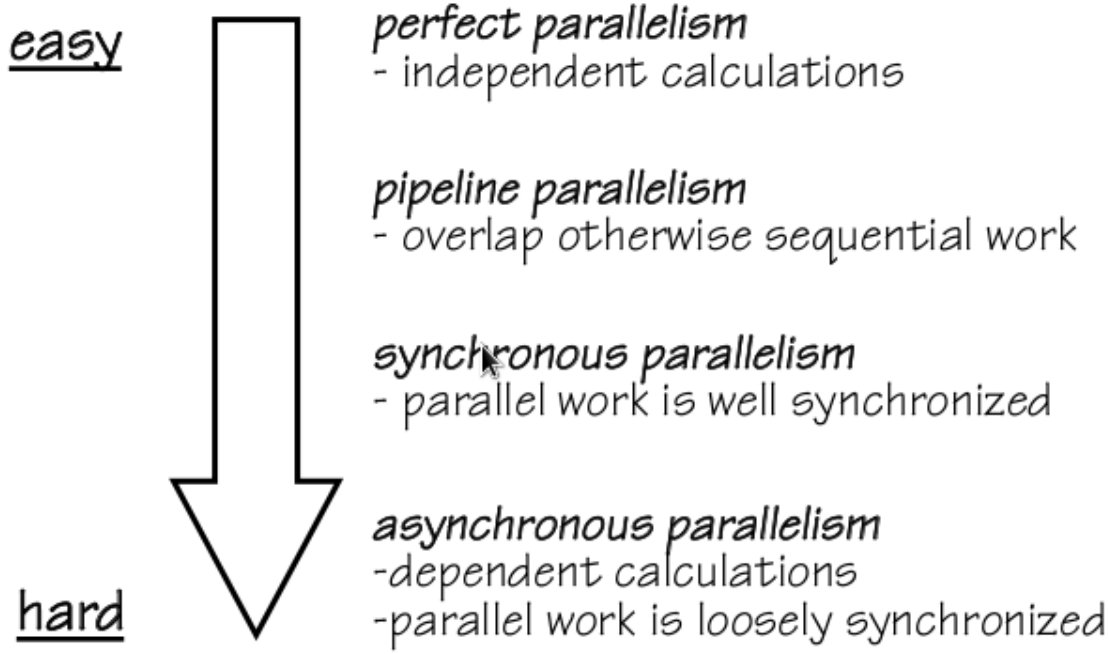
Program Structure

Structure of the problem dictates the ease with which we can implement parallel solutions easy



Parallel Granularity

Granularity

A measure of the amount of processing performed before communication between processes is required.

Parallelism

- Fine Grained
  - constant communication necessary
  - best suited to shared memory environments
- Coarse Grained
  - significant computation performed before communication is necessary
  - ideally suited to message-passing environments
- Perfect
  - no communication necessary

HPC Programming Models

Languages

- serial
  - C, C++, Fortran
- threaded (shared memory)
  - OpenMP, pthreads
- message passing (distributed memory)
  - MPI, PGAS (UPC, Coarray Fortran)
- accelerator (GPU, FPGA)
  - CUDA, OpenCL, OpenACC
  - Starting to be able to program GPUs with OpenMP 4.x

HPC Systems

HPC Software Stack

- Typically GNU/Linux
- non-interactive batch processing using a queuing system scheduler
- software packages and versions usually available as “modules”
- Parallel filesystem (GPFS,Lustre)

Outline

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Serial Jobs

- SciNet is primarily a parallel computing resource. (Parallel here means OpenMP and MPI, not many serial jobs.)

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- Nonetheless, if you can make efficient use of the resources using serial runs and get good science done, that's good too.
- Users need to utilize whole nodes by running at least 40 serial runs at once.

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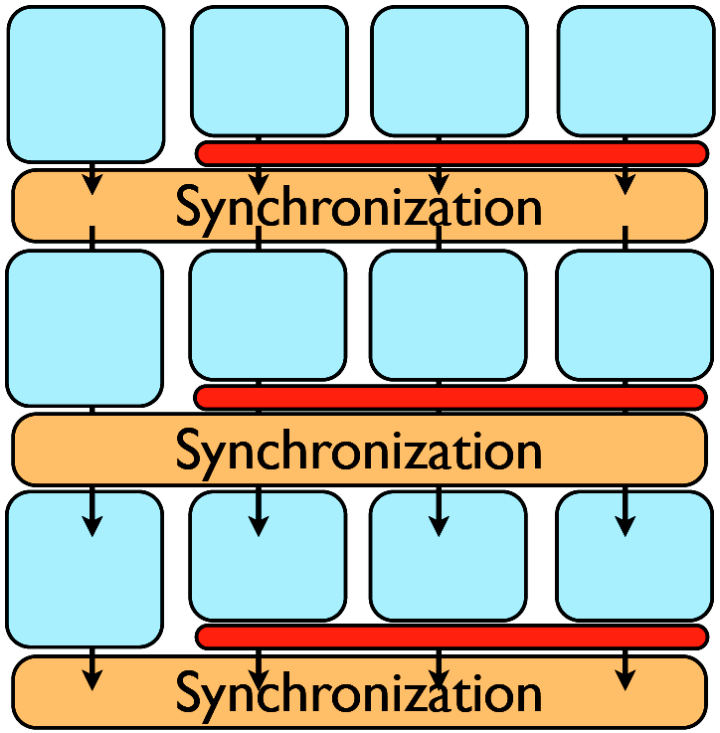
Easy case: serial runs of equal duration

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=1:00:00
cd $SLURM_SUBMIT_DIR
(cd rundir1; ./dorun1) &
(cd rundir2; ./dorun2) &
(cd rundir3; ./dorun3) &
(cd rundir4; ./dorun4) &
(cd rundir5; ./dorun5) &
(cd rundir6; ./dorun6) &
(cd rundir7; ./dorun7) &
...
(cd rundir40; ./dorun40) &
wait # or all runs get killed immediately
```

Hard case: serial runs of unequal duration

Different runs may not take the same time: **load imbalance**.



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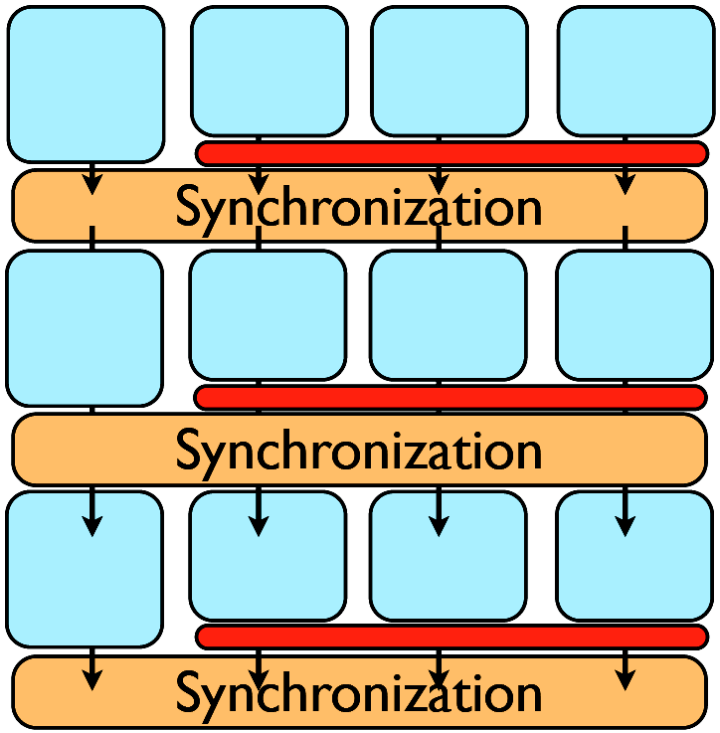

- Want to keep all 40 cores on a node busy.
- Or even 80 virtual cores on a node (HyperThreading).
- ⇒ GNU Parallel can do this

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GNU Parallel

- GNU parallel is a a tool to run multiple (serial) jobs in parallel. *As parallel is used within a Niagara job, we'll call these* **subjobs**.
- It allows you to keep the processors on each 40-core node busy, if you provide enough subjobs.
- GNU Parallel can use multiple nodes as well.

On the Niagara cluster:

- GNU parallel is accessible on the Niagara in the module gnu-parallel:

```
$ module load gnu-parallel/20180322
```

GNU Parallel Example

SETUP

- A serial c++ code 'mycode.cc' needs to be compiled.

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GNU Parallel Example

SETUP

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- It needs to be run 200 times with different parameters, 1 through 200.

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- 40 subjobs of this code fit into a Niagara compute node's memory.

GNU Parallel Example

SETUP

- A serial c++ code 'mycode.cc' needs to be compiled.
- It needs to be run 200 times with different parameters, 1 through 200.
- The parameters are given as a command line argument.
- 40 subjobs of this code fit into a Niagara compute node's memory.
- Each serial run on average takes $\sim$ 2 hour.

GNU Parallel Example

```
$
```

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GNU Parallel Example

```
$ cd $SCRATCH/example
$
```

GNU Parallel Example

```
$ cd $SCRATCH/example
$ module load intel/18.0.2
$
```

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GNU Parallel Example

```
$ cd $SCRATCH/example
$ module load intel/18.0.2
$ icpc -O3 -xHost mycode.cc -o myapp
$
```

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GNU Parallel Example

```
$ cd $SCRATCH/example

$ module load intel/18.0.2

$ icpc -O3 -xHost mycode.cc -o myapp

$ cat subjob.lst
   mkdir run001; cd run001; ../myapp 1 > out
   mkdir run002; cd run002; ../myapp 2 > out
   ...
   mkdir run200; cd run200; ../myapp 200 > out

$
```

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GNU Parallel Example

```
$ cd $SCRATCH/example

$ module load intel/18.0.2

$ icpc -O3 -xHost mycode.cc -o myapp

$ cat subjob.lst
   mkdir run001; cd run001; ../myapp 1 > out
   mkdir run002; cd run002; ../myapp 2 > out
   ...
   mkdir run200; cd run200; ../myapp 200 > out

$ cat NiaJob
      #!/bin/bash
      #SBATCH --nodes=1
      #SBATCH --time=12:00:00
      cd $SCRATCH/example
      module load intel/18.0.2 gnu-parallel/20180322
      parallel --jobs 40 < subjob.lst

$
```

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GNU Parallel Example

```
$ cd $SCRATCH/example

$ module load intel/18.0.2

$ icpc -O3 -xHost mycode.cc -o myapp

$ cat subjob.lst
   mkdir run001; cd run001; ../myapp 1 > out
   mkdir run002; cd run002; ../myapp 2 > out
   ...
   mkdir run200; cd run200; ../myapp 200 > out

$ cat NiaJob
      #!/bin/bash
      #SBATCH --nodes=1
      #SBATCH --time=12:00:00
      cd $SCRATCH/example
      module load intel/18.0.2 gnu-parallel/20180322
      parallel --jobs 40 < subjob.lst

$ sbatch  NiaJob
      Submitted batch job 170

$
```

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GNU Parallel Example

```
$ cd $SCRATCH/example

$ module load intel/18.0.2

$ icpc -O3 -xHost mycode.cc -o myapp

$ cat subjob.lst
   mkdir run001; cd run001; ../myapp 1 > out
   mkdir run002; cd run002; ../myapp 2 > out
   ...
   mkdir run200; cd run200; ../myapp 200 > out

$ cat NiaJob
      #!/bin/bash
      #SBATCH --nodes=1
      #SBATCH --time=12:00:00
      cd $SCRATCH/example
      module load intel/18.0.2 gnu-parallel/20180322
      parallel --jobs 40 < subjob.lst

$ sbatch  NiaJob
      Submitted batch job 170

$ ls
      NiaJob    myapp    slurm-170.out    subjob.lst
      run001    run002   run003           run004
      ...
```

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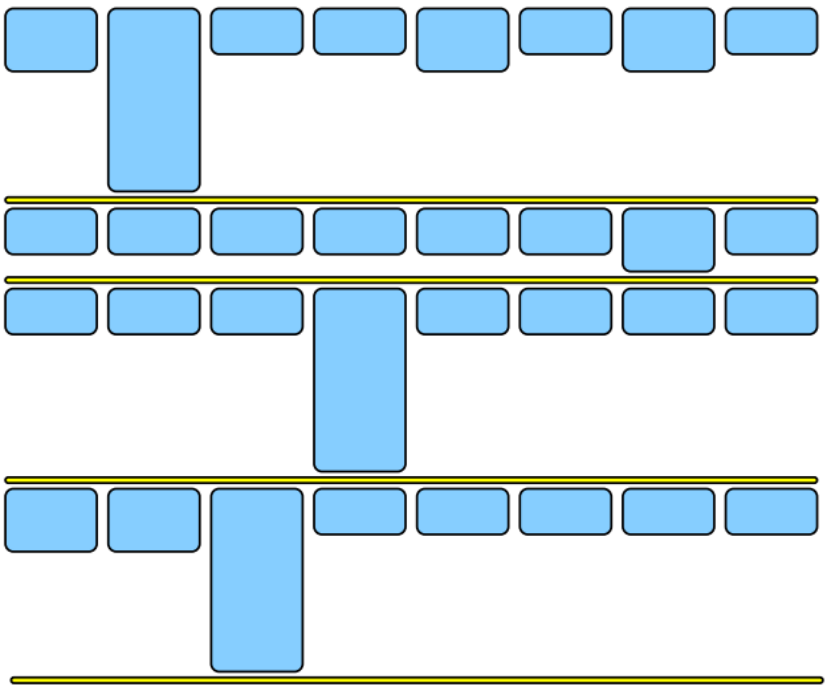
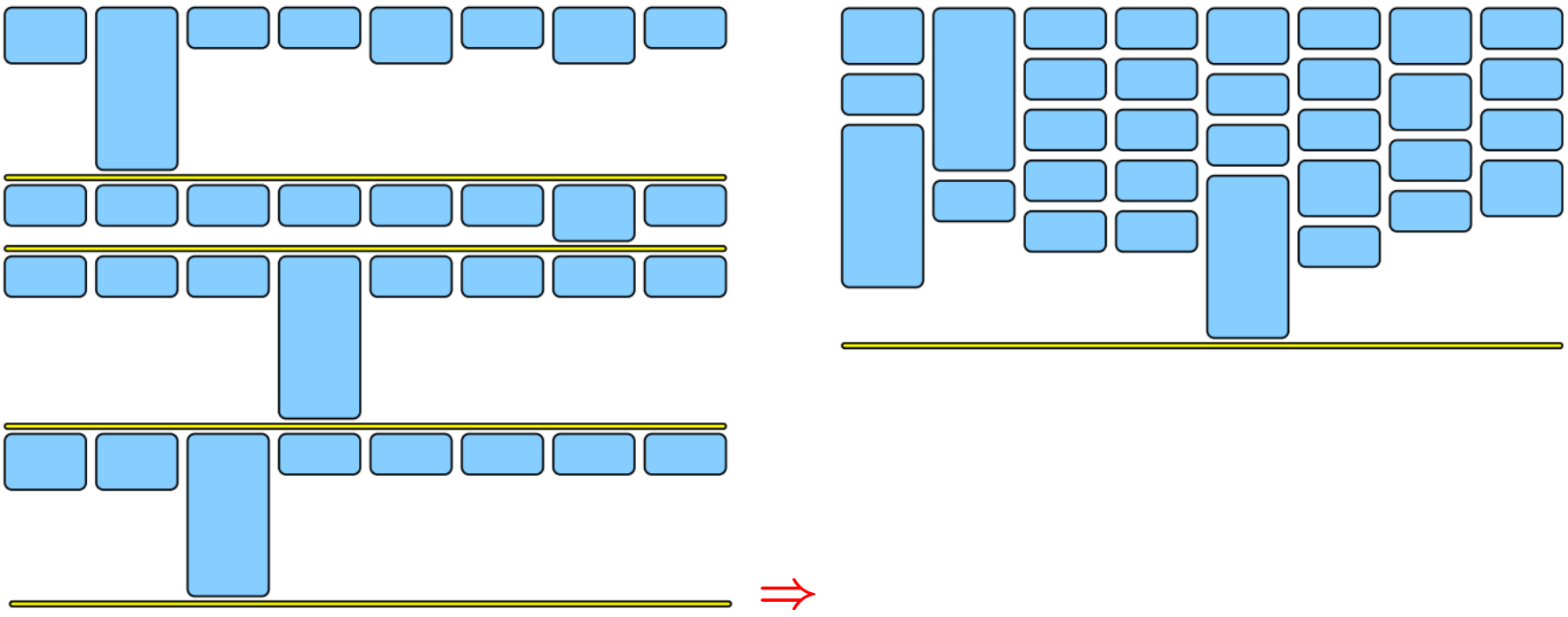
GNU Parallel Example



17 hours
42% utilization

GNU Parallel Example



17 hours
42% utilization

10 hours
72% utilization

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GNU Parallel Details

What else can it do?

- Recover from crashes (joblog/resume options)
- Span multiple nodes

Using GNU Parallel

- docs.scinet.utoronto.ca/index.php/Running_Serial_Jobs_on_Niagara
- www.gnu.org/software/parallel
- www.youtube.com/playlist?list=PL284C9FF2488BC6D1
- O. Tange, GNU Parallel – The Command-Line Power Tool, ;login: The USENIX Magazine, February 2011:42-47.

Outline

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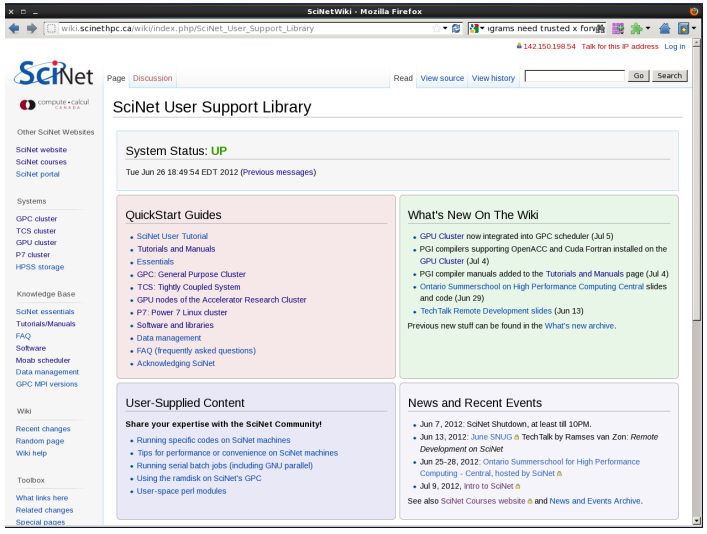
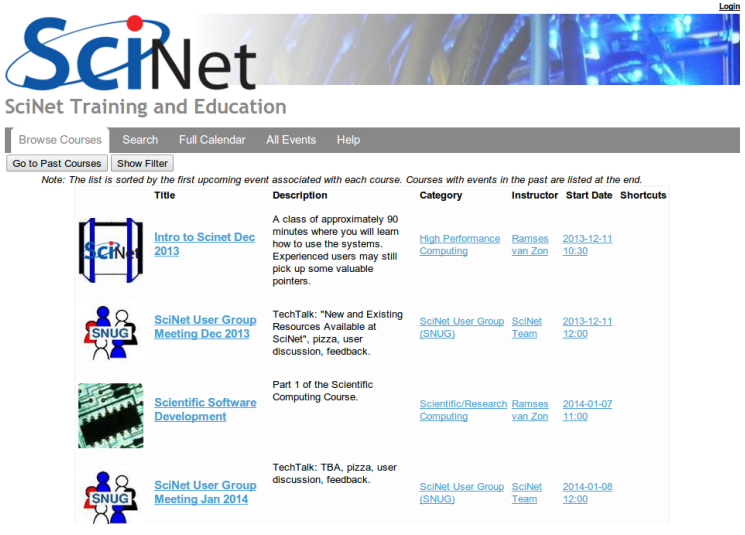
www.scinethpc.ca

docs.scinet.utoronto.ca



https://support.scinet.utoronto.ca/education



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Account Info & Maintenance

https://ccdb.computecanada.ca

- Sign up for a national account
- Request a SciNet account
- Change your password

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EOF

Have a question, or need help?

- Email us at support@scinet.utoronto.ca

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Demo (time permitting)

- Show how to connect to Niagara and submit a job.

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